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by

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Proton-Neutron Pairing Correlations in Atomic Nuclei

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Introduction

In the last years a lot of work has been dedicated to the proton-neutron pairing in nuclei. The revival of this fundamental issue of nuclear structure is related to the recent advances in experimental techniques and to the development of radioactive beams facilities which open the possibility to explore the spectroscopic properties of heavy nuclei close to N=Z line, in which the proton-neutron pairing is expected to play an important role. Thus, in these nuclei the proton-neutron pairing can contribute with additional binding energy which could be essential to their stability and, implicitely, to the location of the proton drip line.

Proton-neutron pairing is also expected to play a significant role in β decays, such as neutrinoless double β decay, which has fundamental consequences for particle physics.

Another nuclear property which can be affected by the proton-neutron pairing is the nuclear mass of nuclei with N≈Z. The experimental masses and their extrapolation far from stability show that the nuclei with N=Z have an additional binding compared with other nuclei. This additional binding energy is commonly referred to as the Wigner energy and it is introduced in the phenomenological mass formulas through a term proportional to |N-Z|. There is a long debate about the origin of the Wigner energy (e.g., see [1] and references quoted therein). Although this issue is not yet settled down, many studies indicate that, at least partially, the Wigner energy is related to the additional binding energy caused by proton-neutron pairing, which becomes stronger in N=Z nuclei [2].

In N=Z nuclei there are, in principle, two channels in which proton-neutron interaction can generate important pairing correlations. Here by pairing correlations we mean the formation of collective pairs which act coherently by forming a pair condensate, such as the BCS condensate. Thus, in N=Z nuclei are commonly considered collective proton-neutron pairs of total angular momentum J=0 and J=1. By analogy with infinite systems, instead of pairs with J=0 and J=1 are sometimes considered pairs with the total spin S=0 and S=1 and total orbital momentum L=0. The total isospin

of the proton-neutron pairs with S=0 (S=1) is T=1 (T=0). More precisely, the proton-neutron (pn) pairs with S=0 correspond to T=1 and $T_z = 0$. The other two components of the isospin T=1 are associated to the neutron-neutron (nn) and proton-proton (pp) pairs. Since the nuclear forces are, with a good approximation, invariant to the isospin projections, one expects that the correlations associated to the nn, pp and np pairs to be of equal strength in N=Z nuclei. All three kinds of collective pairs with T=1 are commonly called isovector pairs. On the other hand, the pairs with S=1 and T=0 are called isoscalar pairs; all of them are proton-neutron pairs with S=1 but with different values of S_z. The isoscalar pairs with $S_z = 0$, in which the protons and the neutrons are in time-conjugate states (have opposite spins) is commonly considered the counterpart of the isovector proton-neutron pairs.

One of the most debated issues in nuclear structure is the competition between the isovector and isoscalar pairing in open shell nuclei with N≈Z. Thus, many studies are trying to answer the following questions: (a) does exist a condensate of isoscalar proton-neutron pairs in the ground state of N=Z nuclei; (b) do the isovector and isoscalar proton-neutron pairing coexist; (c) how persistent are the isovector and isoscalar pn pairing when one moves away of N=Z line; (d) what is the contribution of isoscalar and isovector pairing to Wigner energy; (e) how the isovector and the isoscalar pairing are affecting the excitation spectra and how these spectra can be eventually used to pin down the fingerprints of isoscalar pairing.

From the theoretical point of view, the majority of studies on proton-neutron pairing have been done in the framework of quasiparticle models of BCS-type. Thus, in Refs. [3, 4, 5] the BCS theory for like-particle pairing was extended to treat simultaneously all the components of isovector T=1 pairing, i.e., nn, pp and np pairing. The isoscalar pn pairing, considering only the pn pairs in time-reversed states (i.e., with $J_z = 0$), was first treated in a BCS approach by Goswami and Kisslinger [6]. Later on, making use of a generalized Bogoliubov transformation, the BCS model was extended to include both the isovector and the isoscalar $J_z = 0$ pairing [7, 8]. The most general BCS model, which includes the isovector pairing and all possible J=1 isoscalar pairs, was proposed by Goodman in Ref. [9]. Finally, Goodman has considered a HFB model in which all types of pairing have been treated simultaneously with the mean field properties [10]. With this model it was studied the competition between isovector and isoscalar pn pairing in both ground and excited states [10]. The great advantage of these calculations is that they can be done for any nucleus, allowing a careful study of how various types of pairing correlations depend on the atomic mass and on the relative numbers of protons and neutrons. However, as shown in exactly solvable models [11, 12, 13] and in some schematic calculations [14], the predictions

of the BCS/HFB models on the competition of isovector and isoscalar pairing are affected significantly by the fact that these models do not conserve exactly the particle number and the isospin.

How much are affected the results of BCS calculations by breaking the particle number conservation is quite well-documented for the like-particle pairing. Thus, as has been shown more than 40 years ago by Richardson [15] using the exact solution of the BCS pairing Hamiltonian, the BCS model gives errors of about 40% for the correlation pairing energies in the ground state of nuclei. These large errors can be eventually compensated by fitting the pairing strength to experimental data, such as odd-even mass difference and/or moment of inertia. However, these types of adjustments are difficult to be controlled when the proton-neutron pairing is considered. Indeed, as shown by the majority of BCS/HFB calculations, the balance between various types of pairing is very sensitive to slight changes in the effective pairing forces [10].

For the like-particle pairing the errors of the BCS can be considerably reduced by performing particle-number projected-BCS (PBCS) calculations (for a recent study, see [16]). However, this is not the case for the proton-neutron BCS models. Thus, as shown in a few studies [7, 17], the PBCS calculations with pn pairing give quite large errors. This is mainly because in PBCS applyed for pn pairing there is another symmetry which should be restored: the isospin symmetry. Indeed, as shown in [7], restoring both the particle number and the isospin symmetries the PBCS results become closer to the exact calculations, but not as much as in PBCS calculations for like-particle pairing. To increase further the accuracy one needs to go beyond BCS/PBCS. In Ref.[7] this is done by applying the framework of generator coordinate method (GCM). However, this is an approach which does not give a simple understanding of the types of correlations present in the GCM trial function and, in addition, it is not clear how to extend this method for treating both the isovector and isoscalar pairing.

The alternative approach to treat the pn pairing, presented in this thesis, is to use as building blocks alpha-like quartets instead of Cooper pairs. The fact that one could use quartets in order to restore the isospin symmetry when pn pairing is treated was suggested many years ago by Lane [18].

Alpha-like structures in nuclei are one of the most discussed topics in nuclear physics (see [19] for a recent review), mainly due to its connection to alpha-radioactivity. However, there are also other observables which can be related to the existence of alpha-like structures, such as specific regularities in the masses of light nuclei and in the low-energy excitations of N=Z nuclei [19, 20, 21, 22].

One of the first treatments of pn pairing in terms of alpha-type quar-

tets have been done by Flowers and Vujicic [23]. They have considered a BCS-type condensate of alpha-like quartets in order to describe the isovector pairing in the ground state of N=Z nuclei. Recently in Ref. [24] this model has been extended by considering a BCS-type condensate formed by alpha-like quartets and pairs. However, due to the complication of the variational equations, no applications have been done yet for realistic proton-neutron systems. In fact, a theory of quartet correlations based on a BCS-like function is expected to be not accurate when applied to finite nuclear systems as atomic nuclei. This is due to the large fluctuation in the particle number, which in the case of a BCS-like condensate of quartets is fluctuating in units of four. A different alpha-type approach, conserving the particle number, has been proposed in Ref.[25]. This approach is based on non-collective alpha-like quartets, constructed for each single-particle state. This formalism was applied for a schematic model of two levels and appears difficult to be extended for realistic calculations. An alpha-type condensate constructed with collective quartets was introduced by Talmi in his generalization of the seniority model [26], but he discussed only schematic Hamiltonians which fulfill the generalized seniority rule. First realistic calculations with an alpha condensate have been done in Ref.[27]. In these calculations the collective alpha-type quartet is constructed with all possible intermediate couplings, i.e., considering not only J=0 and J=1 pairs. However, since the use of such complex quartets is a difficult task, the calculations have been done using bosonic type approximations for systems with more than two quartets. A fully bosonic approach for alpha condensate was considered in Ref. [28] using the framework of IBM model.

In the present thesis it is discussed a new quartet model which, compared with the previous models mentioned above, has the following characteristics: 1) the particle number and the total isospin are exactly conserved; 2) it is based on collective quartets built by scattering protons and neutrons in single-particle states around the Fermi levels; 3) the variational equations are solved by preserving exactly the Pauli principle for any number of quartets; 4) the alpha-type quartets are built only with J=0 and J=1 pairs, which make them appropriate for the description of the isovector and the isoscalar pairing but not for all types of correlations contained in a full shell model interaction.

To present the main studies we have done during the PhD programme, we have chosen the following structure of the thesis. First, to set the stage, in the first chapter we review shortly how the proton-neutron pairing is traditionally treated in BCS-type models. Thus, after we recall briefly the BCS model for like-particle pairing, we discuss how BCS is being employed for treating the isovector nn, pp and pn pairing. For that we have used the linearization

method of Ginocchio et al. [32], which is less known than other methods usually presented in textbooks or review papers. This method of treating the isovector pairing presents the great advantage of simplicity, showing clearly that a BCS-theory is not able to take into account properly the pn pairing. Then, in the next section we summarized how both the isovector and the isoscalar pairing are treated in the generalized BCS approach by using the method of Bogoliubov transformation. Finally, making use of the results of Ref.[17], we illustrate how the particle number could be restored in the case of isovector pairing. It is thus concluded that the errors remain still large due to the isospin symmetry breaking.

Then, in the next chapters we discussed the original work we have done during the PhD programme, which has been published in Refs. [29, 30, 31]. Thus, in Chapter II we introduce the quartet condensation model (QCM) for describing the isovector pairing correlations in N=Z nuclei. In Chapter III, we extend the QCM for the nuclei with N>Z and we discuss the coexistence between the quartet condensate and the pair condensate of excess neutrons. Finally, in Chapter IV, we show how QCM can be generalized to include both the isovector and the isoscalar pairing and we discuss the competition between the two pairing modes. In all chapters we present in quite details how are solved the QCM equations by using the method of recurrence relations. In each chapter we present also realistic calculations of the pairing correlation energies for three relevant chains of nuclei with the valence protons and neutrons moving outside the closed cores ^{16}O, ^{40}Ca and ^{100}Sn and we check the accuracy of QCM results by comparing them with the results obtained by the exact shell model calculations.

Chapter 1

Pairing in nuclei: overview of BCS-type models

The existence of pairing correlations in nuclei was suggested more than 50 years ago by Bohr, Mottelson and Pines [33]. Their suggestion was based on the analogy between the gap in the excitation spectra of superconducting metals and the gap in the excitation spectra of even-even nuclei. Since the bare nucleon-nucleon interaction is repulsive at small distances, it was not clear from the begining that a BCS-type condensate can be formed in nuclear systems. This issue was first investigated by Cooper, Mills and Sessler for infinite nuclear matter [34]. They have shown that in nuclear matter a BCS condensate can exist only for densities smaller than the saturation density but their prediction of the pairing gap was not based on a self-consistent microscopic approach. In fact, an ab-initio calculation of the pairing gap in nuclear matter, starting from bare nucleon-nucleon interaction and treating self-consistently the in-medium effects, is still missing [35]. In nuclei, due to finite size effects, the pairing problem is even more difficult to solve self-consistently. Thus, in nuclei it was used from the very begining a phenomenological BCS approach [36], postulating the existence of Cooper pairing and employing effective pairing forces adjusted to observables related to the pairing correlations, such as odd-even mass differences and moments of inertia. The phenomenological BCS model has been applied with a great success in nuclear structure, mainly together with mean field models such as Skyrme-HF, Hartree-Fock-Bogoliubov [37] and Relativistic Mean Field [38]. However, in spite of its success, BCS has an important drawback which introduces important errors when is applied to nuclei: the particle number is conserved only in average. This drawback is mainly noticed when BCS is applied to describe pairing in nuclei with a few nucleons in the valence shell, such as nuclei close to the magic numbers. A better approximation, proposed

already many years ago [39], is the so-called particle-number projected BCS (PBCS) approximation. This approximation is quite easy to apply for a given single-particle spectrum [40], but becomes much more difficult when it is extended to mean field models of Skyrme-HFB type (e.g., see [41] and references quoted therein).

The BCS approximations mentioned above will be shortly reviewed in Section 1.1. They have been applied initially to describe the pairing correlations between neutrons or protons. This is the case of semi-magic nuclei, with only one open shell, or heavy nuclei in which the neutrons and the protons are moving in different valence shells.

A different class of pairing correlations, which we are dealing with in the present thesis, are the pairing correlations between neutrons and protons. These correlations are important in nuclei with the neutrons and protons moving in the same open shell. Usually the proton-neutron pairing is considered in two channels, that is, the isovector and the isoscalar proton-neutron pairing, in which the protons and neutrons are coupled to the total spin S=0 and, respectively, S=1. The isovector and the isoscalar proton-neutron pairing are commonly described with the generalized BCS/HFB models. These models are reviewed in Sections 1.2-1.3.

1.1 BCS approximation for like-particle pairing

For reasons of consistency, we shall start with a short review of the BCS model [42]. Here we shall follow the Ref. [37], in which the BCS approach is presented with notations appropriate for the applications to nuclei.

In nuclei the pairing is associated to a residual two-body force which scatters pairs of nucleons in time-reversed states. Thus, the standard pairing Hamiltonian is written as

$$\hat{H} = \sum_{i}^{\Omega} \epsilon_i (a_i^+ a_i + a_{\bar{i}}^+ a_{\bar{i}}) - \sum_{i>j}^{\Omega} v_{ij} a_i^+ a_{\bar{i}}^+ a_{\bar{j}} a_j. \tag{1.1}$$

In the first term ϵ_i is the energy of the single-particle state i, generated by phenomenological or self-consistent mean field models. The second term is the pairing interaction which scatters the pairs in time-reversed states $(i, \bar{i})$. The most common pairing interaction is the one in which it is considered that the matrix elements of the force do not depend on the states, i.e., $v_{ij} = g$.

In the BCS approximation it is supposed that the ground state of the system can be well described by the trial wave function:

$$|BCS\rangle = \prod_{k>0}(u_k + v_k {a_k}^+ {a_{\bar{k}}}^+)|-\rangle, \tag{1.2}$$

where u_k and v_k are variational parameters and $|-\rangle$ stands for the pair vacuum. From the normalization condition one gets that these parameters should satisfy the relation:

$$|u_k|^2 + |v_k|^2 = 1. \tag{1.3}$$

Explicitely, the BCS state can be written as

$$|BCS\rangle \propto |-\rangle + \sum_{k>0} \frac{v_k}{u_k} {a_k}^+ {a_{\bar{k}}}^+ |-\rangle + \frac{1}{2} \sum_{kk'>0} \frac{v_k v'_k}{u_k u'_k} {a_k}^+ {a_{\bar{k}}}^+ {a_{k'}}^+ {a_{\bar{k'}}}^+ |-\rangle + \cdots. \tag{1.4}$$

It can be seen that the BCS wave function is a superposition of components with various number of pairs. The particle number is conserved only in average by imposing the condition

$$\langle BCS|\hat{N}|BCS\rangle = 2\sum_{k>0} v_k^2 = N. \tag{1.5}$$

One can thus notice that the variational parameters v_k^2 are related to the occupation probabilities of the single-particle levels.

The variational parameters are derived from the minimization of the auxiliary Hamiltonian $H' = H - \lambda N$, where λ is the Lagrange multiplier corresponding to the condition of particle number conservation (in average). One thus gets:

$$v_k^2 = \frac{1}{2}\left(1 \pm \frac{\tilde{\epsilon}_k}{\sqrt{\tilde{\epsilon}_k^2 + \Delta_k^2}}\right), \tag{1.6}$$

$$u_k^2 = \frac{1}{2}\left(1 \pm \frac{\tilde{\epsilon}_k}{\sqrt{\tilde{\epsilon}_k^2 + \Delta_k^2}}\right), \tag{1.7}$$

where $\tilde{\epsilon}_i = \epsilon_i - \lambda$, while

$$\Delta_k = -\sum_{k'} v_{k,k'} u_{k'} v_{k'}, \tag{1.8}$$

is the so-called gap equation.

The equations which define the occupation probabilities together with the gap equation and the equation for the particle number average are the so-called BCS equations. They are a set of non-linear equations which are

solved iteratively up to the convergence. Solving the BCS equations one thus gets the occupation probabilities of the single-particle states and the pairing gap. The latter is commonly associated with the odd-even mass difference. Moreover, the quantities $E_i = \sqrt{\tilde{\epsilon}_i^2 + \Delta_i^2}$ are associated to the quasiparticle excitations of the system. Thus, taking into account that an even system is described by an even number of quasiparticle excitations, it can be seen that 2Δ (considering that the gap does not depend on the state) can be associated to the minimal energy necessary to excite a paired even system.

The BCS model can be also formulated in terms of the Bogoliubov quasiparticles defined as

$$\alpha_k^+ = u_k a_k^+ - v_k a_{\bar{k}}, \tag{1.9}$$

$$\alpha_{\bar{k}}^+ = u_k a_{\bar{k}}^+ + v_k a_k. \tag{1.10}$$

The new quasiparticle operators α_k^+ are also fermionic operators satisfying the anti-commutation relations:

$$\{\alpha_k, \alpha_{k'}\} = 0; \quad \left\{\alpha_k, \alpha_{k'}^+\right\} = \delta_{kk'}. \tag{1.11}$$

As we shall discuss below, the Bogoliubov transformation is particularly suited to generalize the BCS model in order to treat the proton-neutron pairing.

By construction, the BCS theory does not conserve exactly the particle number. A theory of Cooper pairing which conserves exactly the particle number is the so-called particle-number projected-BCS (PBCS) [39, 43]. In its simplest formulation, it amounts in keeping from the BCS wave function (1.4) only the component with the right number of particles. Thus, one gets

$$|PBCS\rangle \propto (\Gamma^+)^{N_{pair}}|-\rangle, \tag{1.12}$$

where $\Gamma^+ = \sum_i x_i a_i^+ a_{\bar{i}}^+$ is the operator which creates a collective Cooper pair. The parameters x_i are determined variationally from the minimization of the pairing Hamiltonian with the $|PBCS\rangle$ wave function.

We end this section with a few comments related to the accuracy of BCS and PBCS approximations for like-particle pairing. The accuracy of these models can be probed by the exact solution of the pairing Hamiltonian, given by Richardson [15] many years ago. Thus, the exact wave function for the ground state of the pairing Hamiltonian (1.1) with $v_{ij} = g$ is given by

$$|\Psi\rangle = \prod_{\nu=1}^{N_{pair}} B_\nu^+|-\rangle, \tag{1.13}$$

where N_{pair} is the number of pairs, while the operators B^+_ν are

$$B^+_\nu = \sum_i \frac{1}{2\epsilon_i - E_\nu} a^+_i a^+_{\bar{i}}. \tag{1.14}$$

These operators depend on the parameters E_ν which are determined solving the set of non-linear equations:

$$\frac{1}{g} - \sum_j \frac{1}{2\epsilon_j - E_\nu} + \sum_{\mu \neq \nu} \frac{2}{E_\mu - E_\nu} = 0. \tag{1.15}$$

The parameters E_ν are related to the ground state energy of the system, E, through the relation $E = \sum_\nu E_\nu$.

From Eq. (1.13) one can see that the exact solution is not a product of identical collective pairs, as in the BCS and PBCS approximations. The question is how accurate are the predictions of these approximations relative to the exact solution. To discuss this issue we use the results of Ref.[16].

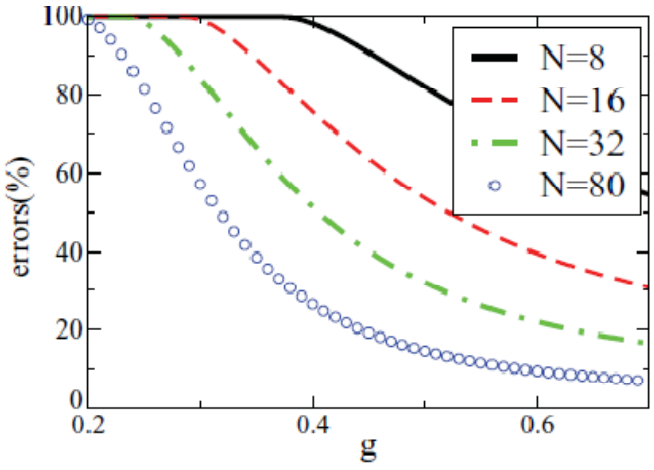

Figure 1.1: Errors in correlation energies for the BCS model. The results are given for a system of N particles distributed in N equally-spaced and double-degenerate levels. The strength g of the force and the correlation energy are given in units of single-particle energies. This figure is taken from Ref. [16].

Thus, in Fig. 1.1 are presented the errors of BCS approximation relative to the exact results for the pairing correlation energy defined by:

$$E_{corr}(g) = E_{HF} - E(g), \tag{1.16}$$

where E_{HF} is the ground state energy of the system in the HF state while $E(g)$ is the energy containing the pairing correlations. The results presented

in Fig. 1.1 correspond to a system of N particles distributed in N equally-spaced and double-degenerate single-particle levels. The results are given for all coupling regimes, starting from weak to the strong coupling. For the physical values of the pairing strength (e.g., $g \approx 0.7$ for N=16) one can see that the BCS approximation gives very large errors for the correlation energies, of about 40%. Increasing the particle number to N=80, but renormalizing the strength as for N=16 (in this case the strength is going from 0.7 to about 0.25), does not improve the accuracy of BCS. In fact, BCS becomes exact only in the thermodynamic limit, which is quite far for small systems such as nuclei.

Going from BCS to PBCS the errors in correlation energies are reduced drastically. This can be seen in Fig. 1.2. For instance, for N=16 and g=0.7 the errors drop from about 40% to less than 5%. On the other hand, one observes that for N=80 and g=0.25 the error of PBCS is still very large. This shows that PBCS does not work properly if it is applied for states very far from the Fermi level. This fact can be understood from the structure of the exact solution. Indeed, only the pairs B_ν built mainly upon states close to the Fermi level can be considered approximatively identical in structure and forming a PBCS type condensate.

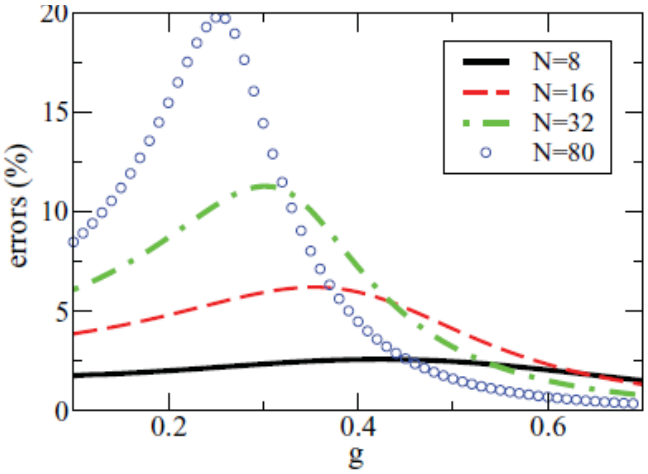

Figure 1.2: The same as in Fig. 1.1 but for PBCS approximation.

1.2 Isovector proton-neutron pairing in the BCS approximation

In nuclei with neutrons and protons in the same major shell one can have collective neutron-neutron (nn) and proton-proton (pp) Cooper pairs with J=0. In addition, due to the isospin invariance of the nuclear forces, one expects to have also important correlations coming from proton-neutron (pn) pairs of J=0. In fact, in N=Z nuclei (nuclei with equal number of protons and neutrons) the nn, pp and pn pairing should generate the same amount of pairing correlations. Since these pairs have the isospin T=1, they are referred to as isovector pairs.

The isovector pairing is commonly described within the BCS approximation generalized to include on equal footing nn, pp and np pairs. The BCS equations are obtained either in the framework of Bogoliubov transformation [3], or using the linearization method [32]. The latter method will be reviewed below. This method has the great advantage of reducing the isovector pairing problem to a product of standard BCS functions for neutron and proton-like degrees of freedom.

Thus, following Ref. [32], we start with the isovector pairing Hamiltonian:

$$\begin{gathered}\hat{H} = \sum_{jm} \epsilon_j [a^+_{jm} a_{jm} + b^+_{jm} b_{jm}] \\ -\tfrac{1}{2} \sum_{jj'} G_{jj'} \{ [\sum_m (-)^{j-m} a^+_{jm} a^+_{j-m}] [\sum_{m'} (-)^{j'-m'} a_{j'-m'} a_{j'm'}] \\ + [\sum_m (-)^{j-m} b^+_{jm} b^+_{j-m}] [\sum_{m'} (-)^{j'-m'} b_{j'-m'} b_{j'm'}] \\ + 2 [\sum_m (-)^{j-m} a^+_{jm} b^+_{j-m}] [\sum_{m'} (-)^{j'-m'} b_{j'-m'} a_{j'm'}] \},\end{gathered}$$

where a^+ and b^+ denote, respectively, the neutron and the proton creation operators. The first term is the single-particle Hamiltonian, described by the single-particle energies ϵ_j. The next three terms are the nn, pp and np pairing interactions for the pairs coupled to J=0 and T=1. As can be seen, all the interactions have the same matrix elements $G_{jj'}$, which is a requirement imposed by the isospin invariance of the nucleon-nucleon force (the Coulomb interaction is not considered in the studies discussed in this thesis).

The linearization method for treating the pairing consists in replacing two-body operators by one-body operators according to the Wicks theorem:

$$a^+_i a^+_j a_k a_l \approx \langle a^+_i a^+_j \rangle a_k a_l + a^+_i a^+_j \langle a_k a_l \rangle - \langle a^+_i a_k \rangle a^+_j a_l + a^+_i a_l \langle a^+_j a_k \rangle. \quad (1.17)$$

One can see that in this approximation it is implicitely supposed that the average of two creation or two anihilation operators is non-zero, which is the case of a BCS-like state. Neglecting the one-body terms of the form a^+a,

which can be assimilated into the single-particle Hamiltonian, the isovector pairing Hamiltonian can be written as

$$\begin{gathered}\hat{H} = \sum_{jm} \epsilon_j [a^+_{jm} a_{jm} + b^+_{jm} b_{jm}] \\ -\tfrac{1}{2} \sum_{jm} \Delta_{nj} [(-)^{j-m} a^+_{jm} a^+_{j-m} + (-)^{j-m} a_{j-m} a_{jm}] \\ -\tfrac{1}{2} \sum_{jm} \Delta_{pj} [(-)^{j-m} b^+_{jm} b^+_{j-m} + (-)^{j-m} b_{j-m} b_{jm}] \\ -\tfrac{1}{2} \sum_{jm} \Delta_{npj} [(-)^{j-m} a^+_{jm} b^+_{j-m} + (-)^{j-m} b_{j-m} a_{jm}],\end{gathered}$$

where the pairing gaps Δ are defined by

$$\Delta_{nj} = \sum_{j'} G_{jj'} \langle \sum_m (-)^{j'-m} a_{j'-m} a_{j'm} \rangle, \tag{1.18}$$

$$\Delta_{pj} = \sum_{j'} G_{jj'} \langle \sum_m (-)^{j'-m} b_{j'-m} b_{j'm} \rangle, \tag{1.19}$$

$$\Delta_{npj} = \sum_{j'} G_{jj'} \langle \sum_m (-)^{j'-m} b_{j'-m} a_{j'm} \rangle. \tag{1.20}$$

In Ref. [32] the solution of the linearized Hamiltonian is searched for in a form which does not involve the coupling term ab. To achieve that, it is performed a rotation in the isospin space as follows:

$$\bar{a}_{jm} = cos\phi_j a_{jm} - sin\phi_j b_{jm}, \tag{1.21}$$

$$\bar{b}_{jm} = sin\phi_j a_{jm} + cos\phi_j b_{jm}. \tag{1.22}$$

In the rotated isospin frame the gaps are expressed by:

$$\Delta_{\bar{a}j} = cos^2\phi_j \Delta_{nj} + sin^2\phi_j \Delta_{pj} - sin2\phi_j \Delta_{npj}, \tag{1.23}$$

$$\Delta_{\bar{b}j} = sin^2\phi_j \Delta_{nj} + cos^2\phi_j \Delta_{pj} + sin2\phi_j \Delta_{npj}, \tag{1.24}$$

$$\Delta_{\bar{a}\bar{b}j} = \frac{1}{2} sin2\phi_j \Delta_{nj} - \frac{1}{2} sin2\phi_j \Delta_{pj} + cos2\phi_j \Delta_{npj}. \tag{1.25}$$

Now it can be seen that the ab coupling can be removed by choosing a rotating angle for which $\Delta_{\bar{a}\bar{b}j}$=0. This angle is defined by the equation

$$\frac{cos2\phi_j}{sin2\phi_j} = \frac{\Delta_{pj} - \Delta_{nj}}{2\Delta_{npj}}. \tag{1.26}$$

It can be observed that the rotating angle is expressed in terms of the gaps in the non-rotated frame. For a separable pairing interaction, i.e., $G_{jj'} = g_j g_{j'}$,

the gaps are independent of single-particle state. In this case the rotation angle can be written as:

$$\phi_j = \phi + n_j \frac{1}{2}\pi. \tag{1.27}$$

Since $n_j \neq 0$ brings just a phase, one can consider $\phi_j = \phi$.

Because by applying the linearization method the particle number conservation was broken, it is imposed its conservation in average. However, compared to the BCS for like-particle pairing, here one should impose the conservation in average of both the neutron and proton numbers. Alternatively, one can use two conditions,that is, the average conservation of the total number of particle and of the isospin projection on z axis:

$$\hat{N} = \sum_{jm} (\bar{a}^+_{jm}\bar{a}_{jm} + \bar{b}^+_{jm}\bar{b}_{jm}) = \sum_j (\hat{N}_{\bar{a}j} + \hat{N}_{\bar{b}j}), \tag{1.28}$$

$$\hat{T}_z = \frac{1}{2}\sum cos2\phi_j(\bar{a}^+_{jm}\bar{a}_{jm} - \bar{b}^+_{jm}\bar{b}_{jm}) + \frac{1}{2}\sum sin2\phi_j(\bar{a}^+_{jm}\bar{b}_{jm} + \bar{b}^+_{jm}\bar{a}_{jm}). \tag{1.29}$$

It can be noticed that the average of the total number of particles (protons and neutrons) can be expressed as a sum of the particle operators in the rotated space. This is not the case with the average of the isospin operator, which contains also mixed terms $(\bar{a}, \bar{b})$. Therefore, in Ref.[32] it is used the following operator for imposing the conservation of the isospin average:

$$\hat{\tau} = \frac{1}{2}\sum_j (\hat{N}_{\bar{a}j} + \hat{N}_{\bar{b}j}) = \frac{1}{2}\sum_{jm} (\bar{a}^+_{jm}\bar{a}_{jm} - \bar{b}^+_{jm}\bar{b}_{jm}). \tag{1.30}$$

Using the approximations mentioned above it can be shown that the ground state of the isovector pairing Hamiltonian can be written as a direct product of the BCS wave functions for rotated neutrons and protons, i.e.,

$$|\Psi\rangle = \prod_{jm>0} [U_{\bar{a}j} + (-)^{j-m} V_{\bar{a}j}\bar{a}^+_{jm}\bar{a}^+_{j-m}] \times [U_{\bar{b}j} + (-)^{j-m} V_{\bar{b}j}\bar{b}^+_{jm}\bar{b}^+_{j-m}]. \tag{1.31}$$

So, in the rotated isospin space, the isovector pairing problem is reduced to the solution of two standard BCS equations for the rotated protons and neutrons.

It is important to remember that, at variance with the like-particle pairing, there are here two chemical potentials which should be determined, λ_N and λ_τ, corresponding to the average conservation of the total number of particle and isospin. They are given by the equations:

$$\langle \frac{1}{2}(\hat{N} + 2\hat{\tau})\rangle = \frac{1}{2}(N + 2\tau) = \sum_j (2j+1)V^2_{\bar{a}j}, \tag{1.32}$$

$$\langle\frac{1}{2}(\hat{N}-2\hat{\tau})\rangle=\frac{1}{2}(N-2\tau)=\sum_{j}(2j+1)V_{\bar{b}j}^{2}. \tag{1.33}$$

Of special interest for systems with proton-neutron pairing is the isospin quantum number. The average of the projection of the isospin on z axis can be written as

$$T_z=\langle\Psi|\hat{T}_z|\Psi\rangle=cos2\phi\langle\Psi|\hat{\tau}|\Psi\rangle=(cos2\phi)\tau. \tag{1.34}$$

On the other hand, the average of the total isospin is given by:

$$\langle\Psi|\hat{T}^2|\Psi\rangle=\tau^2+[N-\sum_{j}(2j+1)(V_{\bar{a}j}^{2}+V_{\bar{b}j}^{2})^2]. \tag{1.35}$$

It can be seen that actually τ^2 is not the average of the total isospin of the system. However, taking into account that the second term in the equation above is usually a small quantity, one can consider that

$$\hat{T}^2\cong\tau^2. \tag{1.36}$$

Thus, in this approximation, τ can be interpreted as the average of the total isospin of the system.

The possible values of the isospin put straightforward constraints on the proton-neutron pairing correlations. This is simply seen in the case of even-even N=Z nuclei. These nuclei have T=0 in the ground state. Imposing the conditions T=0 and T_z=0 it can be shown [17] that the system have in this case two independent and excluding solutions i.e., a solution with $\Delta_n=\Delta_p\neq 0$ and $\Delta_{np}=0$ or a solution with $\Delta_n=\Delta_p=0$ and $\Delta_{np}\neq 0$.

Another important case is the one for even-even nuclei with N>Z and mass larger than 40. These nuclei have a ground state with $T=T_z$. As can be seen from Eq. (1.34), this condition can be fulfilled when the rotation angle is zero. Thus, in this case the ground state can be also described as independent BCS condensates of protons and neutrons, without having contributions from proton-neutron pairing.

1.3 Isovector and isoscalar pairing in BCS-like models

In nuclei with neutrons and protons in the same major shell one can have, in addition to the isovector (T=1) pairing, isoscalar (T=0) proton-neutron pairing. The standard T=0 isoscalar pairing refers to the proton-neutron pairs with total angular momentum J=1, or total spin S=1. In principle,

one can have also isoscalar pn pairing with $J > 1$. However, it is expected that, in general, these pairs are less collective than the pairs with J=1.

Both the isovector and isoscalar pairing correlations are commonly described in generalized BCS or HFB models [44]. In this section, following Ref. [10], we summarize the generalized BCS model.

The generalized BCS calculations are done usually with the two-body Hamiltonian

$$\hat{H} = \sum_j e_j C_j^+ C_j + \frac{1}{4} \sum_{ijkl} \langle ij|v_a|kl\rangle C_i^+ C_j^+ C_l C_k, \tag{1.37}$$

where e_j are the single-particle energies and v_a is the antisymmetrized effective interaction. By i are denoted the quantum numbers of the single- particle states, e.g., $nljm\tau$, where $\tau = \pm 1/2$ are the isospin quantum numbers for neutrons and protons. Below it is also used the notation $\alpha = \{nljm\}$ while the proton and neutron states are labelled explicitely by n and p instead of $\tau = \pm 1/2$. The isovector and the isoscalar pairing is studied by considering in the two-body interaction the terms with (T=1,J=0) and (T=0,J=1).

The pairing correlations are commonly treated by the generalized Bogoliubov transformation. For like-particle pairing the special Bogoliubov transformation has the form:

$$\begin{pmatrix} a_\alpha^+ \\ a_{\bar{a}} \end{pmatrix} = \begin{pmatrix} u_\alpha & -v_\alpha \\ v_\alpha & u_\alpha \end{pmatrix} \begin{pmatrix} C_\alpha^+ \\ C_{\bar{a}} \end{pmatrix}, \tag{1.38}$$

where a^+, a are the quasiparticle operators. In order to take into account the proton-neutron pairing, both isovector and isoscalar, the Bogoliubov transformation is extended as follows:

$$\begin{pmatrix} a^+(\alpha) \\ a(\alpha) \end{pmatrix} = \begin{pmatrix} u(\alpha) & -v(\alpha) \\ -v^*(\alpha) & u^*(\alpha) \end{pmatrix} \begin{pmatrix} C^+(\alpha) \\ C(\alpha) \end{pmatrix}, \tag{1.39}$$

where $a^+(\alpha)$ and $C^+(\alpha)$ are vectors with four components:

$$a^+(\alpha) = \begin{pmatrix} a_{\alpha 1}^+ \\ a_{\alpha 2}^+ \\ a_{\bar{\alpha} 1}^+ \\ a_{\bar{\alpha} 2}^+ \end{pmatrix}, \quad C^+(\alpha) = \begin{pmatrix} C_{\alpha p}^+ \\ C_{\alpha n}^+ \\ C_{\bar{\alpha} p}^+ \\ C_{\bar{\alpha} n}^+ \end{pmatrix}. \tag{1.40}$$

The quantities $u(\alpha)$ and $v(\alpha)$ are four-dimensional matrices of the following form:

$$u(\alpha) = u_\alpha I_4, \quad v(\alpha) = \begin{pmatrix} 0 & v_{\alpha 1} & v_{\alpha 2} & v_{\alpha 3} \\ -v_{\alpha 1} & 0 & v_{\alpha 3}^* & -v_{\alpha 2} \\ -v_{\alpha 2} & -v_{\alpha 3}^* & 0 & v_{\alpha 1}^* \\ -v_{\alpha 3} & v_{\alpha 2} & -v_{\alpha 1}^* & 0 \end{pmatrix}. \tag{1.41}$$

$u_\alpha, v_{\alpha 2}$ are real and $v_{\alpha 1}, v_{\alpha 3}$ are complex.

In the generalized BCS the trial wave function is taken as a superposition of all possible isovector and isoscalar pairs and has the expression:

$$|\Phi_0\rangle = \prod_{\alpha>0} \left(u_\alpha + v^*_{\alpha 1} C^+_{\alpha p} C^+_{\alpha n} + v_{\alpha 2} C^+_{\alpha p} C^+_{\bar{\alpha} p} + v^*_{\alpha 3} C^+_{\alpha p} C^+_{\bar{\alpha} n}\right) \left(u_\alpha + v_{\alpha 1} C^+_{\bar{\alpha} p} C^+_{\bar{\alpha} n} - v_{\alpha 2} C^+_{\alpha n} C^+_{\bar{\alpha} n} + v_{\alpha 3} C^+_{\alpha n} C^+_{\bar{\alpha} p}\right) |0\rangle.$$

From the normalization condition of the BCS wave function one gets

$$v^2_\alpha = |v_{\alpha 1}|^2 + |v_{\alpha 2}|^2 + |v_{\alpha 3}|^2, \tag{1.42}$$

where v^2_α plays the role of the occupation probability of the orbital α. The equations for the variational parameters are obtained from the minimization of the average of the pairing Hamiltonian. One thus gets [10]:

$$u_\alpha = \left[\frac{1}{2}[1 + \frac{\epsilon_\alpha - \lambda}{E_\alpha}]\right]^{1/2}, \quad v_\alpha = \left[\frac{1}{2}[1 + \frac{\epsilon_\alpha - \lambda}{E_\alpha}]\right]^{1/2}, \tag{1.43}$$

$$v_{\alpha 1} = -v_\alpha(\Delta^*_{\alpha p,\alpha n}/\Delta_\alpha), \tag{1.44}$$

$$v_{\alpha 2} = -v_\alpha(\Delta_{\alpha p,\bar{\alpha} p}/\Delta_\alpha), \tag{1.45}$$

$$v_{\alpha 3} = -v_\alpha(\Delta^*_{\alpha p,\bar{\alpha} n}/\Delta_\alpha). \tag{1.46}$$

The pairing gaps entering in the expressions above are defined by:

$$\Delta_{\alpha p,\bar{\alpha} p} = \sum_{\beta>0} \langle \alpha\bar{\alpha} T = 1 | v_a | \beta\bar{\beta} T = 1\rangle u_\beta v_{\beta 2}, \tag{1.47}$$

$$Re\ \Delta_{\alpha n,\bar{\alpha} p} = \sum_{\beta>0} \langle \alpha\bar{\alpha} T = 1 | v_a | \beta\bar{\beta} T = 1\rangle u_\beta Re\ v_{\beta 3}, \tag{1.48}$$

$$Im\ \Delta_{\alpha n,\bar{\alpha} p} = \sum_{\beta>0} \langle \alpha\bar{\alpha} T = 0 | v_a | \beta\bar{\beta} T = 0\rangle u_\beta Im\ v_{\beta 3}, \tag{1.49}$$

$$Re\ \Delta_{\alpha p,\alpha n} = \frac{1}{2}\sum_{\beta>0} [\langle \alpha\alpha T = 0 | v_a | \beta\beta T = 0\rangle + \langle \alpha\alpha T = 0 | v_a | \bar{\beta}\bar{\beta} T = 0\rangle] u_\beta Re\ v_{\beta 1}, \tag{1.50}$$

$$Im\ \Delta_{\alpha p,\alpha n} = \frac{1}{2}\sum_{\beta>0} [\langle -\alpha\alpha T = 0 | v_a | \beta\beta T = 0\rangle + \langle \alpha\alpha T = 0 | v_a | \bar{\beta}\bar{\beta} T = 0\rangle] u_\beta Im\ v_{\beta 1}. \tag{1.51}$$

It can be observed that the real part of $\Delta_{\alpha n,\bar{\alpha} p}$ is related to the isovector ($T = 1$) pairing while the imaginary part of $\Delta_{\alpha n,\bar{\alpha} p}$ stands for the isoscalar ($T = 0$) pairing.

The quasiparticle energies can be written, formally, as in the BCS theory for like-particle pairing, i.e.,

$$E_\alpha = [(\epsilon_\alpha - \lambda)^2 + \Delta_\alpha^2]^{1/2}. \tag{1.52}$$

The pairing gap includes now the contributions coming from all types of pairing and has the expression:

$$\Delta_\alpha^2 = |\Delta_{\alpha p,\bar{\alpha} p}|^2 + |\Delta_{\alpha p,\bar{\alpha} n}|^2 + |\Delta_{\alpha p,\alpha n}|^2. \tag{1.53}$$

Finally, the chemical potential is obtained from the average conservation of the particle number. For the systems with equal number of protons and neutrons one thus have:

$$N = Z = 2\sum_{\alpha>0} v_\alpha^2. \tag{1.54}$$

The equations above represent the generalized BCS equations for isovector and isoscalar pairing. As can be seen, they have a much more complicated structure than in the case of like-particle pairing.

The generalized BCS approximation summarized above contains only the pairing correlations obtained from pairs in time-reversed states. A more general theory, which includes pairs in states which are not time-reversed, is the generalized HFB [44]. The generalized HFB has been applied extensively for the study of the competition between the isovector and isoscalar pairing, both in the ground and excited states (e.g., see [10] and the references quoted therein). In many calculations it appears that the isovector and the isoscalar pairing do not coexist together. However, as indicated by some studies (e.g., see [14]), it appears that this conclusion is affected by the fact that HFB does not conserve exactly the particle number and the isospin. The restoration of these two symmetries was never done in the generalized HFB calculations. As an example, in the following section we shall discuss how the particle number restoration affects the BCS results for isovector pairing.

1.4 Isovector pairing in the PBCS approximation

As we have already mentioned in the previous section, the BCS/HFB treatment of proton-neutron pairing has the disavantage of not conserving exactly the particle number and the isospin. The question we shall discuss in this section is how much one can improve the BCS results if one restores the particle number conservation. As an example we take the case of the isovector pairing analysed in Ref. [17] .

Thus, following Ref. [17], we consider the isovector pairing described with a pairing force of constant strength, i.e., a force with all the matrix elements equal to a constant. The corresponding Hamiltonian is:

$$\hat{H} = \sum_{i\tau} \epsilon_i a^+_{i\tau} a_{i\tau} - g \sum_{i,i',\tau} \hat{j}_i \hat{j}_{i'} P^+_{i\tau} P_{i'\tau}, \tag{1.55}$$

where $P^+_{i\tau} = \frac{1}{\sqrt{2}}[a^+_i a^+_{\tilde{i}}]^{01}_{0\tau}$ are the isovector pair creation operators for neutron-neutron ($\tau = 1$), proton-proton ($\tau = -1$) and proton-neutron pairs ($\tau = 0$). This Hamiltonian has the SO(5) symmetry and can be solved exactly by the Richardson-Gaudin method (e.g., see [45]).

The common approximation used to treat the Hamiltonian (1.55) is the BCS. As we have already mentioned in Section 1.2, the BCS gives for the isovector pairing two independent and degenerate solutions, one corresponding to $\Delta_{np} = \Delta$ and $\Delta_n = \Delta_p = 0$ and the other to $\Delta_n = \Delta_p = \Delta$ and $\Delta_{np} = 0$ (see [17]).

Restoring the particle number in BCS is commonly done with the projection operators. In the case of isovector pairing this approach is rather complicated and does not provide a simple understanding of the projected wave function. As an alternative, in Ref.[17] are constructed explicitely the PBCS wave functions corresponding to the two degenerate BCS solutions mentioned above. Thus, for a nucleus with N=Z it is considered a PBCS wave function formed by N collective proton-neutron pairs of the following form:

$$|PBCS0\rangle = \frac{1}{N!}(\Gamma^+_0)^N |0\rangle, \tag{1.56}$$

where Γ^+_0 is the collective neutron-proton pair operator defined by

$$\Gamma^+_0 = \sum_{i=1}^{L} x_i P^+_{i0}. \tag{1.57}$$

For even-even N=Z nuclei there is another possibility to construct a PBCS state, which corresponds to the second BCS solution. This wave function is

a product of two PBCS condensates, one formed by nn pairs and the other by pp pairs, i.e.

$$|PBCS1\rangle = \frac{1}{(M!)^2}(\Gamma_n^+\Gamma_p^+)^M|0\rangle, \tag{1.58}$$

where M is the number of nn and pp pairs, i.e., $M = N/2 = Z/2$. Γ_n^+ and Γ_p^+ are the collective pair operators for neutrons and protons:

$$\Gamma_n^+ = \sum_{i=1}^{L} y_i P_{i1}^+, \quad \Gamma_p^+ = \sum_{i=1}^{L} y_i P_{i-1}^+. \tag{1.59}$$

Since for N=Z nuclei the system is unchanged by the interchange of protons and neutrons, the mixing amplitudes for the proton and neutron collective pairs are the same.

To determine the mixing amplitudes it is minimized the energy functional $\langle PBCS|H|PBCS\rangle$ under the condition $\langle PBCS|PBCS\rangle = 1$. The calculations are done using the method of recurrence relations.

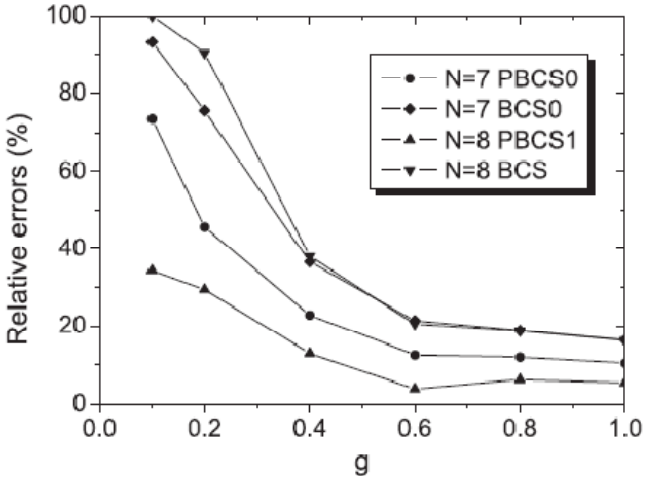

Figure 1.3: Errors for the correlation energies obtained in PBCS0, PBCS1 and BCS approximations. The results are given for seven and eight pn pairs distributed in N equidistant and double-degenerate levels. This figure is taken from Ref. [17].

As a numerical example, here we summarize some results of Ref.[17] obtained for systems formed by N pn pairs distributed in N double-degenerate single-particle states with energies $\epsilon_i = i$ (i=1,2,..,N). Thus, in Fig. 1.3 are shown the errors of PBCS1 and PBCS0 approximations as well as of BCS model relative to the exact results for pairing correlation energies. The results are given for seven and eight pn pairs and for a pairing strength g going

from 0 to 1, covering all the pairing regimes, from weak to strong coupling. The pairing strength and the correlation energies are measured in units of single-particle levels spacing.

Two important informations can be extracted from Fig. 1.3. Thus, one can see that for N=8 (N=7) the PBCS1 (PBCS0) gives much better results than BCS. In fact, the two PBCS solutions, PBCS1 and PBCS0, give the minimum energy for N=even and, respectively, N=odd systems. One can thus conclude that for even systems the minimum is obtained with the PBCS1 solution which does not contain pn pairs. Moreover, from Fig. 1.3 one can also notice that the errors associated to the PBCS1 solution are much larger than in the case of PBCS applied to the like-particle pairing [16]. The reason is that for isovector pairing there is another symmetry broken, in addition to the particle number, the isospin symmetry. Indeed, as can be seen from the structure of PBCS1 condensate, this state has the right number of particles, the right value of the isospin projection on z axis but has not a well-defined total isospin. Isospin restoration is expected to bring additional pairing correlations. However, in order to restore the isospin one should go beyond BCS or PBCS approximations. This is the main issue of this thesis which will be discussed in the next chapters.

Chapter 2

Isovector pairing and quartet condensation in N=Z nuclei

In the previous introductory chapter it was seen that the BCS-type models are not able to describe accurately the proton-neutron pairing correlations in the ground state of even-even self-conjugate nuclei. The main reason why the BCS-type models fail to take into account properly the isovector pairing interaction is the fact that these models are built by independent Cooper pairs of isospin T=1. Thus, since the pairs are independent, the total isospin is not well-defined. The restoration of the total isospin can be achieved by using standard projection techniques. Because the isospin is a vector operator, this task is much more complicated than projecting out the particle number. However, the most important drawback is that the standard isospin projection is not able to improve too much the accuracy of the pairing calculations compared to the generalized BCS or PBCS models (see the discussion in Section 2.3 below). This failure shows that one needs to go beyond the BCS-type models. One alternative, explored in Ref. [46], is to do generator coordinate method (GCM) calculations using as generating function the projected-BCS state and as dynamical coordinates the neutron and the proton gaps. The GCM approximation seems to work very well for N=Z nuclei [46]. However, due to the complicated structure of the trial wave function, the GCM calculations do not provide a clear understanding of the types of correlations induced by the isovector pairing correlations. Moreover, GCM becomes very difficult to apply for nuclei with N>Z and for treating both the isovector and isoscalar pairing correlations.

The alternative which we follow here is to treat the isovector pairing not in terms of Cooper pairs but with alpha-like quartets formed by two neutrons and two protons coupled to the total isospin T=0. The idea of using quartets for treating the isovector pairing is quite old [18]. However, the quartets have

been used either with BCS-type states which violate the particle number conservation [23, 24] or with approximations which are strictly valid only for a limited number of quartets [27]. Here we present the quartet model we have proposed in Ref. [30].

2.1 Quartet condensation model: formalism

The physical system we are going to describe in terms of quartets is formed by a certain number of protons and neutrons distributed in a set of single-particle states of energies ϵ_i and interacting by an isovector pairing force. The corresponding Hamiltonian is:

$$\hat{H} = \sum_i \epsilon_i (N_i^\nu + N_i^\pi) + \sum_{i,j} V_{ij} \sum_{\tau=0,\pm 1} P_{i,\tau}^+ P_{j,\tau}. \tag{2.1}$$

In the single-particle term the operators N_i^ν and N_i^π are, respectively, the neutron and proton number operators. The pairing interaction is written in terms of the pair operators:

$$P_{i,\tau}^+ = [a_i^+ a_{\bar{i}}^+]_{M=0,\tau}^{J=0,T=1}. \tag{2.2}$$

As usual, by $\bar{i}$ we denote the time conjugate of the state i. By τ we label the three projections of the isospin T=1 corresponding to nn ($\tau = 1$), pp ($\tau = -1$) and pn ($\tau = 0$) pairs. Explicitely, the three pair operators are:

$$P_{i,1}^+ = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2j_i+1}} \sum_{m_i} (-)^{j_i - m_i} \nu_{j_i m_i}^+ \nu_{j_i - m_i}^+, \tag{2.3}$$

$$P_{i,-1}^+ = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2j_i+1}} \sum_{m_i} (-)^{j_i - m_i} \pi_{j_i m_i}^+ \pi_{j_i - m_i}^+, \tag{2.4}$$

$$P_{i,0}^+ = \frac{1}{\sqrt{2j_i+1}} \sum_{m_i} (-)^{j_i - m_i} \nu_{j_i m_i}^+ \pi_{j_i - m_i}^+. \tag{2.5}$$

It can be seen that all these operators describe pairs with J=0.

As we have mentioned, the solution of the pairing Hamiltonian will be formulated in terms of quartets. Let's first introduce the following non-collective quartet operators formed by two isovector pairs coupled to the total isospin T=0:

$$A_{ij}^+ = [P_i^+ P_j^+]^{T=0} = \frac{1}{\sqrt{3}} (P_{i,1}^+ P_{j,-1}^+ + P_{i,-1}^+ P_{j,1}^+ - P_{i,0}^+ P_{j,0}^+). \tag{2.6}$$

Then, with the non-collective quartets we define a collective quartet operator

$$A^+ = \sum_{i,j} x_{ij} A^+_{ij}. \tag{2.7}$$

In analogy to the PBCS models, we construct now a condensate of collective quartets of the form:

$$|\Psi\rangle = (A^+)^{n_q}|0\rangle. \tag{2.8}$$

The question we address is whether or not this state can reasonably describe the isovector pairing interaction in the ground state of even-even self-conjugate nuclei. As in the BCS model, we treat as active only the nucleons from a finite energy window around the Fermi level. More precisely, in the quartet condensate written above n_q is the number of quartets which can be formed by the pairing active protons and neutrons and the "vaccum" state $|0\rangle$ denotes the non-active nucleons from a closed core with equal number of protons and neutrons. Thus, we shall further denote by N and Z the number of pairing active neutrons and protons and by n_q the number of quartets, equal to (N+Z)/4 (with N=Z=even).

Since the collective quartet has the same quantum numbers as the alpha particle (i.e., ^{4}He), the quartet A^+ will be called alpha-like. It should however be kept in mind that the quartet A^+ is not a boson operator and it does not describe a bound system such as an alpha particle.

The collective quartet is defined in terms of the mixing amplitudes x_{ij}, which should be determined variationally. The calculations can be greatly simplified if one supposes that the amplitudes are separable in indices i and j, i.e.,

$$x_{i,j} \approx x_i x_j. \tag{2.9}$$

In this approximation the quartet operator A^+ can be written as:

$$A^+ = \sum_i x_i P^+_{i,1} \sum_j x_j P^+_{j,-1} + \sum_i x_i P^+_{i,-1} \sum_j x_j P^+_{j,1} - \sum_i x_i P^+_{i,0} \sum_j x_j P^+_{j,0}. \tag{2.10}$$

In the equation above we recognize the collective nn ($\tau = 1$), pp ($\tau = -1$) and pn ($\tau = 0$) pair operators we have introduced in the previous chapter (see Section 1.4), i.e.,

$$\Gamma^+_\tau = \sum_i x_i P^+_{i\tau}. \tag{2.11}$$

It can be seen that the mixing amplitudes for the collective pair operators are the same for nn, pp and pn pairs, which is the consequence of the isospin invariance and of the equality between neutrons and protons.

Thus, assuming the separability of the mixing amplitudes, the collective quartet operator can be written as

$$A^+ = 2\Gamma_1^+\Gamma_{-1}^+ - (\Gamma_0^+)^2. \tag{2.12}$$

Using this expression of the collective quartet operator, the quartet condensate gets the form:

$$|\Psi\rangle = (2\Gamma_1^+\Gamma_{-1}^+ - \Gamma_0^{+2})^{n_q}|0\rangle = \sum_k \binom{n_q}{k} (-1)^{n_q-k} 2^k (\Gamma_1^+\Gamma_{-1}^+)^k \Gamma_0^{+2(n_q-k)}|0\rangle. \tag{2.13}$$

One can observe that the quartet condensate is a coherent superposition, defined by the binomial expansion, of condensates formed by nn, pp and np collective pairs. By construction, the quartet condensate has a total angular momentum J=0 and a total isospin T=0. It is worth mentioning that in principle there are many other possibilities to form a wave function with the same quantum numbers, i.e., J=0,T=0. The question is whether or not the particular coupling scheme of the quartet condensate is able to take into account a large part of the correlations induced by the isovector pairing.

In the expansion (2.13) one can notice that there are two terms, corresponding to the two PBCS approximations discussed in the previous chapter (see Section 1.4). Thus, one is formed by a product of nn and pp pairs, i.e.,

$$|PBCS1\rangle = (\Gamma_1^+\Gamma_{-1}^+)^{M=N/2=Z/2}|0\rangle. \tag{2.14}$$

The other one is formed by a condensate of neutron-proton pairs and has the form

$$|PBCS0\rangle = (\Gamma_0^+)^{N=A/2}|0\rangle. \tag{2.15}$$

As we have discussed in Section 1.4, the condensate PBCS1, when it is taken alone, gives for N=Z=even systems more correlations than the condensate PBCS0. It means that, at the level of PBCS, there are no proton-neutron pairing correlations in the trial wave function. One might think that pn correlations can be introduced by using a linear combination between the states PBCS1 and PBCS0. This is not the case because this combination does not restore the isospin symmetry, except for the case N=Z=2. In fact, as seen from Eq. (2.13), in order to obtain an isospin conserving function one needs to combine all possible PBCS1 and PBCS0 condensates compatible with the particle number conservation and the binomial expansion.

The alpha-type condensate (2.13) is considered as a trial wave function for the ground state of even-even N=Z systems interacting with isovector pairing and described by the Hamiltonian (2.1). The condensate depends on the

mixing amplitudes x_i which define the collective pair operators. The mixing amplitudes are considered as variational parameters which are determined by minimizing the average of the Hamiltonian $\langle\Psi|\hat{H}|\Psi\rangle$ with the constraint $\langle\Psi|\Psi\rangle = 1$. The average of the Hamiltonian and the norm are calculated using the method of recurrence relations which is presented in Section 2.2 below.

2.2 Quartet condensation model: recurrence relations for N=Z nuclei

The calculation of the average of the Hamiltonian and of the norm with the quartet condensation wave function is not a trivial task. The calculation scheme we have used is based on the set of auxiliary states:

$$|n_1, n_2, n_3\rangle = \Gamma_1^{+n_1}\Gamma_{-1}^{+n_2}\Gamma_0^{+n_3}|0\rangle. \tag{2.16}$$

As seen above, these states are defined for an arbitrary number of nn, pp and pn collective pairs. Similar auxiliary states, but for non-collective pairs, have been introduced in Ref. [25]. It can be observed that the condensate (2.13) can be written as a particular superposition of these states:

$$|\Psi\rangle = \sum_k \binom{n_q}{k} (-1)^{n_q-k} 2^k |k, k, 2(n_q-k)\rangle. \tag{2.17}$$

To calculate the matrix elements of the Hamiltonian in the basis defined by the auxiliary states one needs to know how the operators of the SO(5) algebra, which defines the isovector pairing Hamiltonian, act on these states. These operators are the isovector pair operators $P^+_{i,\tau}$, the particle number operators and the isospin operators

$$T_{i,\tau} = [a_i^+ a_i]^{J=0,T=1}_{M=0,\tau}. \tag{2.18}$$

The commutation relations of these basic operators, which are necessary to do the calculation of the matrix elements, are given below. Thus, it can be shown that the pair operators satisfy the following commutation relations:

$$[P_{i,0}, P^+_{j,0}] = \delta_{ij}(1 - \frac{1}{2}N_{i,0}),\ [P_{i,0}, P^+_{j,1}] = \delta_{ij}T_{i,1},\ [P_{i,0}, P^+_{j,-1}] = -\delta_{ij}T_{i,-1}, \tag{2.19}$$

$$[P_{i,1}, P^+_{j,1}] = \delta_{ij}(1 - N_{i,1}),\ [P_{i,1}, P^+_{j,-1}] = 0,\ [P_{i,-1}, P^+_{j,-1}] = \delta_{ij}(1 - N_{i,-1}). \tag{2.20}$$

One can thus see that in order to close the SO(5) algebra one needs to include also the commutations involving the particle number and the isospin operators. These commutators are:

$$[N_{i,0}, P^+_{j,\tau}] = 2\delta_{ij} P^+_{i,\tau}, \tag{2.21}$$

$$[N_{i,\pm1}, P^+_{j,\mp1}] = 0,\ [N_{i,\pm1}, P^+_{j,\pm1}] = 2\delta_{ij} P^+_{i,\pm1},\ [N_{i,\pm1}, P^+_{j,0}] = \delta_{ij} P^+_{i,0}. \tag{2.22}$$

$$[T_{i,\pm1}, P^+_{j,0}] = \mp\delta_{ij} P^+_{i,\pm1},\ [T_{i,1}, P^+_{j,-1}] = -\delta_{ij} P^+_{i,0},\ [T_{i,-1}, P^+_{j,1}] = \delta_{ij} P^+_{i,0}. \tag{2.23}$$

With the commutation relations given above and using the operator equality

$$[A, B^M] = MB^{M-1}[A, B] + \frac{M(M-1)}{2}[[A, B], B]B^{M-2}, \tag{2.24}$$

one can deduce the following actions:

$$P_{i,1}|n\rangle = -\tfrac{n_3(n_3-1)}{2} x_i^2 P^+_{i,-1}|n_1 n_2 n_3 - 2\rangle + n_1 x_i |n_1 - 1 n_2 n_3\rangle$$
$$-n_1 n_3 x_i^2 P^+_{i,0}|n_1 - 1 n_2 n_3 - 1\rangle - n_1(n_1-1) x_i^2 P^+_{i,1}|n_1 - 2 n_2 n_3\rangle,$$

$$P_{i,-1}|n\rangle = -\tfrac{n_3(n_3-1)}{2} x_i^2 P^+_{i,1}|n_1 n_2 n_3 - 2\rangle + n_2 x_i |n_1 n_2 - 1 n_3\rangle$$
$$-n_2 n_3 x_i^2 P^+_{i,0}|n_1 n_2 - 1 n_3 - 1\rangle - n_2(n_2-1) x_i^2 P^+_{i,-1}|n_1 n_2 - 2 n_3\rangle,$$

$$P_{i,0}|n\rangle = n_3 x_i |n_1 n_2 n_3 - 1\rangle - \tfrac{n_3(n_3-1)}{2} x_i^2 P^+_{i,0}|n_1 n_2 n_3 - 2\rangle$$
$$-n_1 n_2 x_i^2 P^+_{i,0}|n_1 - 1 n_2 - 1 n_3\rangle - n_1 n_3 x_i^2 P^+_{i,1}|n_1 - n_2 n_3 - 1\rangle$$
$$-n_2 n_3 x_i^2 P^+_{i,-1}|n_1 n_2 - 1 n_3 - 1\rangle,$$

$$N_{i,0}|n\rangle = 2n_3 x_i P^+_{i,0}|n_1 n_2 n_3 - 1\rangle + 2n_1 x_i P^+_{i,1}|n_1 - 1 n_2 n_3\rangle + 2n_2 x_i P^+_{i-1}|n_1 n_2 - 1 n_3\rangle, \tag{2.25}$$

$$N_{i,1}|n\rangle = n_3 x_i P^+_{i,0}|n_1 n_2 n_3 - 1\rangle + 2n_1 x_i P^+_{i,1}|n_1 - 1 n_2 n_3\rangle, \tag{2.26}$$

$$N_{i,-1}|n\rangle = n_3 x_i P^+_{i,0}|n_1 n_2 n_3 - 1\rangle + 2n_2 x_i P^+_{i,-1}|n_1 n_2 - 1 n_3\rangle, \tag{2.27}$$

$$T_{i,1}|n\rangle = -n_2 x_i P^+_{i,0}|n_1 n_2 - 1 n_3\rangle - n_3 x_i P^+_{i,1}|n_1 n_2 n_3 - 1\rangle, \tag{2.28}$$

$$T_{i,-1}|n\rangle = n_1 x_i P^+_{i,0}|n_1 - 1 n_2 n_3\rangle + n_3 x_i P^+_{i,-1}|n_1 n_2 n_3 - 1\rangle. \tag{2.29}$$

The equations above can be further used to calculate the matrix elements of the Hamiltonian. For illustration we give here the matrix elements for the

two-body operator $P^+_{i,1}P_{j,1}$ which defines the pairing interaction for neutrons. The matrix elements are:

$$\begin{gathered}
\langle n'_1n'_2n'_3|P^+_{i,1}P_{j,1}|n_1n_2n_3\rangle = n_1x_j\langle n_1-1n_2n_3|P_{i,1}|n'_1n'_2n'_3\rangle \\
-x_ix_j^2(n'_1n_1n_3\langle n_1-1n_2n_3-1|P_{j,0}|n'_1-1n'_2n'_3\rangle \\
+n'_1n_1(n_1-1)\langle n_1-2n_2n_3|P_{j,1}|n'_1-1n'_2n'_3\rangle \\
+\tfrac{1}{2}n'_1n_3(n_3-1)\langle n_1n_2n_3-2|P_{j,-1}|n'_1-1n'_2n'_3\rangle) \\
+x_i^2x_j^2[n'_1n'_3n_1n_3[\langle n'_1-1n'_2n'_3-1|P^+_{j,0}P_{i,0}|n_1-1n_2n_3-1\rangle \\
+\delta_{ij}(\langle n'_1-1n'_2n'_3-1|n_1-1n_2n_3-1\rangle \\
-\tfrac{1}{2}\langle n'_1-1n'_2n'_3-1|N_{i,0}|n_1-1n_2n_3-1\rangle)] \\
+n'_1(n'_1-1)n_1n_3[\langle n'_1-2n'_2n'_3|P^+_{j,0}P_{i,1}|n_1-1n_2n_3-1\rangle \\
-\delta_{ij}\langle n'_1-2n'_2n'_3|T_{i,-1}|n_1-1n_2n_3-1\rangle] \\
+\tfrac{1}{2}n'_3(n'_3-1)n_1n_3[\langle n'_1n'_2n'_3-2|P^+_{j,0}P_{i,-1}|n_1-1n_2n_3-1\rangle \\
+\delta_{ij}\langle n'_1n'_2n'_3-2|T_{i,1}|n_1-1n_2n_3-1\rangle] \\
+n'_1n'_3n_1(n_1-1)[\langle n_1-2n_2n_3|P^+_{i,0}P_{j,1}|n'_1-1n'_2n'_3-1\rangle \\
-\delta_{ij}\langle n_1-2n_2n_3|T_{i,-1}|n'_1-1n'_2n'_3-1\rangle] \\
+n'_1(n'_1-1)n_1(n_1-1)[\langle n'_1-2n'_2n'_3|P^+_{j,1}P_{i,1}|n_1-2n_2n_3\rangle \\
+\delta_{ij}(\langle n'_1-2n'_2n'_3|n_1-2n_2n_3\rangle-\langle n'_1-2n'_2n'_3|N_{i,1}|n_1-2n_2n_3\rangle)] \\
+\tfrac{1}{2}n'_3(n'_3-1)n_1(n_1-1)\langle n'_1n'_2n'_3-2|P^+_{j,1}P_{i,-1}|n_1-2n_2n_3\rangle \\
+\tfrac{1}{2}n'_1n'_3n_3(n_3-1)[\langle n_1n_2n_3-2|P^+_{i,0}P_{j,-1}|n'_1-1n'_2n'_3-1\rangle \\
+\delta_{ij}\langle n_1n_2n_3-2|T_{i,1}|n'_1-1n'_2n'_3-1\rangle] \\
+\tfrac{1}{2}n'_1(n'_1-1)n_3(n_3-1)\langle n_1n_2n_3-2|P^+_{i,1}P_{j,-1}|n'_1-2n'_2n'_3\rangle \\
+\tfrac{1}{4}n'_3(n'_3-1)n_3(n_3-1)[\langle n'_1n'_2n'_3-2|P^+_{j,-1}P_{i,-1}|n_1n_2n_3-2\rangle \\
+\delta_{ij}(\langle n'_1n'_2n'_3-2|n_1n_2n_3-2\rangle-\langle n'_1n'_2n'_3-2|N_{i,-1}|n_1n_2n_3-2\rangle)]].
\end{gathered}$$

It can be seen that the matrix elements of $P^+_{i,1}P_{j,1}$ depend on the matrix elements of the basic SO(5) operators $P_{i,\tau}$, $P^+_{i,\tau}$, $N_{i,\tau}$ and $T_{i,\tau=\pm1}$, but also on the matrix elements of all other two-body operators $P^+_{i,\tau}P_{j,\tau'}$. In particular, it can be observed that in order to evaluate recursively the matrix elements of the pairing interaction one needs also to calculate the matrix elements of two-body operators with $\tau \neq \tau'$, which are not operators appearing in the two-body pairing interaction. This fact makes the calculations not trivial.

To calculate the norm of the quartet condensate one needs the overlaps of the auxiliary states, i.e., $\langle n'_1n'_2n'_3|n_1n_2n_3\rangle$. They are expressed in terms of the matrix elements of the pair operators. For example one can write

$$\begin{gathered}
\langle n'_1n'_2n'_3|n_1n_2n_3\rangle = \textstyle\sum_i x_i\langle n'_1n'_2n'_3|P^+_{i,1}|n_1-1n_2n_3\rangle \\
= \textstyle\sum_i x_i\langle n_1-1n_2n_3|P_{i,1}|n'_1n'_2n'_3\rangle^*.
\end{gathered}$$

Similar relations can be written in terms of the operators $P_{i,-1}$ and $P_{i,0}$. Since the recurrence relations for the pair operators involve the overlaps of the auxiliary states, the latter should be iterated together with the former.

In applying the recursive method one needs to provide the initial starting values for the matrix elements. They should be analytically derived as functions of the mixing amplitudes. As an example, we give below the matrix elements between auxiliary states with zero and one collective pair. For the state with no pairs we use the notation $|-\rangle = |n_1 = 0, n_2 = 0, n_3 = 0\rangle$. It should be remembered that here the number of pairs refers to the pairing active particles, usually the ones outside the double magic core N=Z. We start by presenting an example of how the calculations are done for the matrix elements of $P_{i,0}$:

$$\langle -|P_{i,0}|001\rangle = \langle -|[P_{i,0}, \Gamma_0^+]|-\rangle = \sum_j x_j \langle -|[P_{i,0}, P_{j,0}^+]|-\rangle$$
$$= \sum_j x_j \langle -|\delta_{ij}(1 - \tfrac{1}{2}N_{i,0})|-\rangle = \sum_j x_j \delta_{ij} \langle -|-\rangle - \sum_j x_j \tfrac{1}{2} \langle -|N_{i,0}|-\rangle = x_i.$$

In the same way are calculated the following matrix elements:

$$\langle -|P_{i,1}|100\rangle = \langle -|P_{i,-1}|010\rangle = x_i, \tag{2.30}$$

$$\langle 001|T_{i,1}|010\rangle = \langle 100|T_{i,1}|001\rangle = -x_i^2, \tag{2.31}$$

$$\langle 001|N_{i,0}|001\rangle = \langle 010|N_{i,0}|010\rangle = \langle 100|N_{i,0}|100\rangle = 2x_i^2. \tag{2.32}$$

For the calculation of the norm we need the initial value:

$$\langle 001|001\rangle = \sum_i x_i^2. \tag{2.33}$$

Finally, below we give the initial values for the matrix elements of the pairing interactions:

$$\langle 001|P_{i,0}^+ P_{j,0}|001\rangle = \langle 010|P_{i,-1}^+ P_{j,-1}|010\rangle = \langle 100|P_{i,1}^+ P_{j,1}|100\rangle = x_i x_j. \tag{2.34}$$

Starting from the initial values of the matrix elements one gets, recursively, the matrix elements of the Hamiltonian and the norm for the actual number of pairs. Then, from the matrix elements in the auxiliar basis states one gets the average of the Hamiltonian on the quartet condensate wave function, i.e., $E(x) =< \Psi|H|\Psi >$. Finally, the functional $E(x)$ is minimized numerically with the constraint $< \Psi|\Psi >= 1$. The details about the numerical calculations are given in Appendix. As a result, we get the ground state energy and the occupation probabilities of the single-particle states.

2.3 Application of quartet condensation model to N=Z nuclei

The calculation scheme presented above can be applied for describing the isovector pairing correlations in any even-even self-conjugate nuclei. One important question is how accurate are the predictions of the quartet condensation model. In order to analyse this issue we take as examples systems for which exact shell model calculations can be done. Thus, we analyse the isovector pairing correlations for three types of N=Z nuclei with the valence nucleons moving outside the closed cores ^{16}O, ^{40}Ca and ^{100}Sn, considered as inert. For these nuclei we have done two types of calculations, supposing that the nucleons are moving in a spherical or in a deformed mean field. We start by presenting the calculations done in the spherical symmetry. In this case the isovector pairing force is extracted from the (T=1, J=0) part of the standard shell model (SM) interactions. More precisely, we consider the following input for the interaction and the single-particle energies:

(1) nuclei with the core ^{16}O: the universal sd-shell interaction (USDB) [47] and the single-particle energies: $\epsilon_{1d_{5/2}}$=-3.926, $\epsilon_{2s_{1/2}}$=-3.208 and $\epsilon_{1d_{3/2}}$=2.112;

(2) nuclei with the core ^{40}Ca: the monopole-modified Kuo-Brown interaction (KB3G) [48] and the energies: $\epsilon_{1f_{7/2}} = 0.0$, $\epsilon_{2p_{3/2}}$=2.0, $\epsilon_{2p_{1/2}}$=4.0 and $\epsilon_{1f_{5/2}}$=6.5;

(3) nuclei with the core ^{100}Sn: the effective G-matrix interaction from Ref. [49] and the energies: $\epsilon_{2d_{5/2}}$=0.0, $\epsilon_{1g_{7/2}}$=0.2, $\epsilon_{2d_{3/2}}$=1.5 and $\epsilon_{3s_{1/2}}$=2.8. Here and above, all single-particle energies are expressed in MeV.

In order to be able to do exact SM calculations, for the second and the third type of nuclei are neglected, respectively, the single-particle levels $1g_{9/2}$ and $1h_{11/2}$. However this limitation is not necessary for doing QCM calculations, which can be performed in the full valence shells.

It is worth mentioning that for zero values of the single-particle energies ϵ_i and for an interaction of constant strength the isovector pairing Hamiltonian has an analytical solution. Thus, the ground state energy is given by

$$E = -g[N(\Omega + \frac{3}{2} - \frac{1}{2}N) - \frac{1}{2}T_z(T_z - 1) - \delta(T_z + 1)], \tag{2.35}$$

where N is the number of pairs, Ω is the number of the states, T_z is the projection of the isospin and δ is 0 for even-even ($T = T_z$) systems and 1 for odd-odd ($T = T_z + 1$) systems [13]. We have used this particular case for testing the recurrence relations and the numerical code which solves the QCM equations.

The QCM results obtained for the three types of nuclei are presented in

Table 2.1. In this table are given the correlation pairing energies defined by:

$$E_{corr} = E_0 - E, \tag{2.36}$$

where E_0 is the energy calculated without the pairing interaction and E is the energy of the ground state with the isovector pairing included. In brackets are given the errors relative to the shell model results, shown in the second column. In the last two columns are given the correlation energies obtained with the two PBCS approximations defined in Eqs. (2.14, 2.15).

Table 2.1: Correlation energies calculated for spherical single-particle states. The results are given for the exact shell model diagonalizations (SM), for the quartet condensation model (QCM) and for the two PBCS approximations defined in Eqs. (2.14, 2.15). In brackets are given the errors relative to the exact SM results.

	SM	QCM	PBCS1	PBCS0
^{20}Ne	9.173	9.170 (0.033%)	8.385 (8.590%)	7.413 (19.187%)
^{24}Mg	14.460	14.436 (0.166%)	13.250 (8.368%)	11.801 (18.389%)
^{28}Si	15.787	15.728 (0.374%)	14.531 (7.956%)	13.102 (17.008%)
^{32}S	15.844	15.795 (0.309%)	14.908 (5.908%)	13.881 (12.389%)
^{44}Ti	5.973	5.964 (0.151%)	5.487 (8.134%)	4.912 (17.763%)
^{48}Cr	9.593	9.569 (0.250%)	8.799 (8.277%)	7.885 (17.805%)
^{52}Fe	10.768	10.710 (0.539%)	9.815 (8.850%)	8.585 (20.273%)
^{104}Te	3.831	3.829 (0.052%)	3.607 (5.847%)	3.356 (12.399%)
^{108}Xe	6.752	6.696 (0.829%)	6.311 (6.531%)	5.877 (12.959%)
^{112}Ba	8.680	8.593 (1.002%)	8.101 (6.670%)	13.064 (13.064%)

As it can be seen, the approximation PBCS1 gives much smaller errors than PBCS0. Since PBCS1 is composed only from nn and pp pairs, it can be concluded that the PBCS approximation is not able to take into account the pn correlations. This fact was already noticed for the case of a schematic isovector pairing model (see Section 1.4).

The most important fact which can be seen in Table 2.1 is that QCM gives very small errors, under 1% for all the isotopes considered. We can thus see that even in the case of ^{32}S, where there are four quartets above ^{16}O, QCM gives excellent results. Excellent results are also obtained for the nuclei with the core ^{100}Sn.

An interesting question is whether or not the very good accuracy of QCM is just a consequence of particle number and isospin symmetry restoration.

To answer this question we made a comparison between the QCM results and the results given by the particle number and isospin projected-BCS state

$$|PBCS(N,T)\rangle = \hat{P}_T \hat{P}_N |BCS\rangle, \tag{2.37}$$

where $\hat{P}_T$ is the isospin projection operator and $\hat{P}_N$ is the particle number projection operator. For comparison we have used the results provided by PBCS(N,T) for the isotope ^{52}Fe, given in Ref. [46]. These calculations have been done with an isovector pairing interaction of constant strength ($g = -24/A$, A being the mass of the nucleus) acting on spherical single-particle states (for details, see Ref.[46]). Thus, with PBCS(N,T) is obtained for ^{52}Fe a correlation energy of 7.63 MeV. The exact result is 8.29 MeV, which shows that PBCS(N,T) is a rather poor approximation. On the other hand, QCM gives for the correlation energy the value 8.25 MeV, which is a very accurate result. From this example one can conclude that the standard isospin projection is not accurate enough for getting a good description of the isovector pairing correlations. But the most important conclusion which can be drawn from this comparison is the fact that, compared to PBCS(N,T), QCM takes into account additional correlations, of four-particle type.

In the calculations presented up to now we have treated the N=Z nuclei as being spherical. This is not a very good approximation because for these nuclei the deformation plays a very important role. The question we are addresing now is how the deformation is going to affect the quartet correlations. To analyse this issue we have considered that the deformation can be treated reasonably well working in the intrinsic frame of an axially deformed mean field. The deformed mean field and the corresponding single-particle energies have been calculated with the Skyrme-HF approach using the Skyrme force SLy4 [50] and neglecting the Coulomb interaction.

For the QCM calculations done with the single-particle energies generated by the axially deformed mean field we have used an isovector pairing force of seniority type with a constant pairing strength $g = -24/A$. Since the pairing force is of finite range, we have employed in the QCM calculations only a limited number of single-particle states around the Fermi level. More precisely, in the QCM calculations done for the three types of nuclei shown in Table 2.1 we have used the lowest seven, nine, and, respectively, ten deformed single-particle levels above the closed cores. The results obtained for the deformed nuclei are given in Table 2.2. As can be seen from this table QCM gives very accurate results for deformed single-particle states as well.

Thus, we conclude that QCM gives very accurate results for the correlation energies induced by the isovector pairing interaction in the ground state of N=Z nuclei. It should be also mentioned that the QCM calculations are

Table 2.2: Correlation energies calculated for axially deformed single-particle states.

	SM	QCM	PBCS1	PBCS0
^{20}Ne	6.55	6.539 (0.168%)	5.752 (12.183%)	4.781 (27.008%)
^{24}Mg	8.423	8.388 (0.415%)	7.668 (8.963%)	6.829 (18.924%)
^{28}Si	9.661	9.634 (0.279%)	9.051 (6.314%)	8.384 (13.218%)
^{32}S	10.263	10.251 (0.117%)	9.854 (3.985%)	9.372 (18.682%)
^{44}Ti	3.147	3.142 (0.159%)	2.750 (12.615%)	2.259 (28.217%)
^{48}Cr	4.248	4.227 (0.494%)	3.854 (9.275%)	3.423 (19.421%)
^{52}Fe	5.453	5.426 (0.495%)	5.033 (7.702%)	4.582 (15.973%)
^{104}Te	1.084	1.082 (0.184%)	0.964 (11.070%)	0.832 (23.247%)
^{108}Xe	1.870	1.863 (0.374%)	1.697 (9.264%)	1.514 (19.037%)
^{112}Ba	2.704	2.688 (0.592%)	2.532 (6.361%)	2.184 (19.230%)

very fast (a few minutes run on an ordinary laptop) and applicable for nuclei with more active nucleons and levels than can be treated by the present SM codes.

Chapter 3

Isovector pairing and quartet condensation in nuclei with N>Z

3.1 Extension of quartet condensation model (QCM) for N>Z nuclei

As we have seen in the previous chapter, the isovector pairing corelations in the ground state of N=Z nuclei are very accurately described by a quartet condensate. The issue we address here is how the quartet condensate model can be extended for nuclei which have in the valence space a different number of protons and neutrons. In these nuclei only a part of the active nucleons can be coupled in quartets. The question is whether or not the quartets can coexist with the excess neutrons or protons and how the latter can be properly treated.

The Hamiltonian describing the isovector pairing in nuclei with different number of protons and neutrons in the valence shell is the same as for N=Z systems. Thus, as in the previous chapter, we consider the Hamiltonian:

$$\hat{H} = \sum_i \epsilon_i (N_i^\nu + N_i^\pi) + \sum_{i,j} V_{ij} \sum_\tau P_{i,\tau}^+ P_{j,\tau}, \tag{3.1}$$

where, as above, the pair operators are given by

$$P_{i,\tau}^+ = [a_i^+ a_{\bar{i}}^+]_{M=0,\tau}^{J=0,T=1}. \tag{3.2}$$

We shall now proceed to extend the QCM to nuclei with $N \neq Z$. Here we consider the case of nuclei with N>Z, with both N and Z even numbers. The nuclei with $Z > N$ can be treated in a similar way.

First we suppose that all the proton-neutron (pn) pairs which can be formed in the valence space are coupled to form a quartet condensate. Thus, as in the case of N=Z nuclei we introduce the quartet collective operator:

$$A^+ = 2\Gamma_1^+\Gamma_{-1}^+ - (\Gamma_0^+)^2. \tag{3.3}$$

With this quartet operator we then construct a quartet condensate which includes all the pn pairs from the valence space.

Next, we consider that the remaining number of neutrons are described by a PBCS condensate of collective neutron-neutron (nn) pairs:

$$\tilde{\Gamma}_1^+ = \sum_i y_i P_{i1}^+. \tag{3.4}$$

Finally, we suppose that the valence nucleons are described by a product of two condensates, of quartets and of neutron pairs in excess. This state is written as

$$|\Psi\rangle = (\tilde{\Gamma}_1^+)^{n_N}(A^+)^{n_q}|0\rangle = (\tilde{\Gamma}_1^+)^{n_N}(2\Gamma_1^+\Gamma_{-1}^+ - \Gamma_0^{+2})^{n_q}|0\rangle. \tag{3.5}$$

In the equation above $n_N = (N-Z)/2$ is the number of neutron pairs which cannot be included in the quartets and $n_q = (N-2n_N+Z)/4$ is the maximum number of quartets which can be constructed with the valence nucleons. It is worth mentioning that the state (3.5) becomes the exact solution of the isovector pairing Hamiltonian when all the single-particle levels are degenerate [13].

In writing the state for the N>Z system we considered that the neutron collective pairs in excess, described by the operator $\tilde{\Gamma}_1^+$, have a structure which is different from the structure of the collective neutron pairs included in the quartets,i.e.

$$\Gamma_1^+ = \sum_i x_i P_{i1}^+. \tag{3.6}$$

This is a requirement imposed by the Pauli principle in the HF limit.

The mixed condensate (3.5) has the total isospin given by the neutrons in excess (since the isospin of the quartets is T=0), i.e., $T = T_z = n_N$. This is, in fact, the isospin expected for the ground state of even-even nuclei with N>Z and N+Z> 40.

As in the case of N=Z nuclei, the mixed condensate (3.5) contains two terms which can be associated to the PBCS approximation. Thus, one term contains a product of two pair condensates, one of nn pairs in excess and one of pn pairs:

$$|PBCS0\rangle = (\tilde{\Gamma}_1^+)^{n_N}(\Gamma_0^+)^{2n_q}|0\rangle. \tag{3.7}$$

The other term is a product of two condensates formed by nn and pp pairs

$$|PBCS1\rangle = (\tilde{\Gamma}_1^+)^{N/2}(\Gamma_{-1}^+)^{Z/2}|0\rangle. \tag{3.8}$$

These two states represent the generalization of the PBCS approximation for the systems with N>Z. In contrast to the system with N=Z, the state PBCS0 contains both like-particle pairs (nn) and pn pairs.

The state (3.5) is used here to describe the isovector pairing correlations in nuclei with N>Z. The parameters x_i and y_i are determined variationally imposing the minimization of the average of the pairing Hamiltonian. Since now the number of variational parameters is twice than in the case of N=Z nuclei, the QCM calculations become much more difficult. How the recurrence relations can be extended to solve the QCM equations for N>Z systems is shown in the next section.

3.2 Solution of QCM equations: recurrence relations

The solutions of the QCM equations are obtained by expanding the condensate wave function (3.5) in the basis of auxiliary states

$$|n_1 n_2 n_3 n_4\rangle = \Gamma_1^{+n_1}\Gamma_{-1}^{+n_2}\Gamma_0^{+n_3}\tilde{\Gamma}_1^{+n_4}|0\rangle. \tag{3.9}$$

It can be seen that, compared to the case of N=Z nuclei, the auxiliary states depend on a new index, n_4, associated to the neutron pairs in excess relative to the proton pairs.

As in the case of N=Z nuclei, one first needs to evaluate how the basic operators, i.e., pair operators, particle number operator, and isospin operators, act on the auxiliary states. For that we use the same commutation relations as the ones given in the previous chapter. As an example, we give below the action of the neutron pair operator $P_{i,1}$ on the auxiliary state (3.9):

$$\begin{gathered}
P_{i,1}|n_1 n_2 n_3 n_4\rangle = -n_3(n_3-1)x_i^2 P_{i,-1}^+|n_1 n_2 n_3 - 2 n_4\rangle \\
+n_1 x_i|n_1 - 1 n_2 n_3 n_4\rangle - 2n_1 n_3 x_i^2 P_{i,0}^+|n_1 - 1 n_2 n_3 - 1 n_4\rangle \\
-2n_1(n_1-1)x_i^2 P_{i,1}^+|n_1 - 2 n_2 n_3 n_4\rangle + n_4 y_i|n_1 n_2 n_3 n_4 - 1\rangle \\
-2n_3 n_4 x_i y_i P_{i,0}^+|n_1 n_2 n_3 - 1 n_4 - 1\rangle \\
-4n_1 n_4 x_i y_i P_{i,1}^+|n_1 - 1 n_2 n_3 n_4 - 1\rangle - 2n_4(n_4-1)y_i^2 P_{i,1}^+|n_1 n_2 n_3 n_4 - 2\rangle.
\end{gathered}$$

It can be observed that, because the extra neutron pairs, this equation is more complicated than the corresponding equation for N=Z systems.

Next we show how the matrix elements of two-body operators are calculated. We take as example the matrix elements of the operator $P^+_{i,1}P_{j,1}$. They can be written as

$$\langle m, m_4|P^+_{i,1}P_{j,1}|n, n_4\rangle = \langle m, m_4|P^+_{i,1}P^{(n)}_{j,1}|n, n_4\rangle + n_4 y_j\langle m, m_4|P^+_{i,1}|n, n_4 - 1\rangle$$
$$-2n_4 y_j\langle m, m_4|P^+_{i,1}N^{(n)}_{j,1}|n, n_4 - 1\rangle - 2n_4(n_4 - 1)y^2_j\langle m, m_4|P^+_{i,1}P^+_{j,1}|n, n_4 - 2\rangle.$$

In the equation above we abreviated the set of indices n_1, n_2, n_3 by n. The operators labeled by $P^{(n)}$ means that they act only on the set of the first three indices and not on the forth one. This action can be calculated using the relations given for N=Z systems. As an illustration, we show the results for the first term of the previous equation:

$$\begin{aligned}\langle m, m_4|P^+_{i,1}P^{(n)}_{j,1}|n, n_4\rangle = &-n_3(n_3 - 1)x^2_j\langle m, m_4|P^+_{i,1}P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle\\ &+n_1x_j\langle m, m_4|P^+_{i,1}|n_1 - 1n_2n_3, n_4\rangle\\ &-2n_1n_3x^2_j\langle m, m_4|P^+_{i,1}P^+_{j,0}|n_1 - 1n_2n_3 - 1, n_4\rangle\\ &-2n_1(n_1 - 1)x^2_j\langle m, m_4|P^+_{i,1}P^+_{j,1}|n_1 - 2n_2n_3, n_4\rangle.\end{aligned}$$

From this expression we choose again the first term for illustrating the next step of the derivation. This time we have to act with $P^+_{i,1}$ on the left side of the matrix element. One thus gets:

$$\begin{aligned}&\langle m, m_4|P^{+(n)}_{i,1}P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle =\\ &-m_3(m_3 - 1)x^2_i\langle m_1m_2m_3 - 2, m_4|P_{i,-1}P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle\\ &m_1x_i\langle m_1 - 1m_2m_3, m_4|P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle\\ &-2m_1m_3x^2_i\langle m_1 - 1m_2m_3 - 1, m_4|P_{i,0}P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle\\ &-2m_1(m_1 - 1)x^2_i\langle m_1 - 2m_2m_3, m_4|P_{i,1}P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle.\end{aligned}$$

Now the final step is to rearrange all the above terms in order to reproduce the matrix elements already known. Thus, the first term from the above equation represents the matrix elements of $P_{i,-1}P^+_{j,-1}$, but what we know actually are the matrix elements of $P^+_{j,-1}P_{i,-1}$. Making use of the commutator between $P_{i,-1}$ and $P^+_{j,-1}$ one obtains

$$\begin{aligned}&\langle m_1m_2m_3 - 2, m_4|P_{i,-1}P^+_{j,-1}|n_1n_2n_3 - 2, n_4\rangle =\\ &\langle m_1m_2m_3 - 2, m_4|P^+_{j,-1}P_{i,-1}|n_1n_2n_3 - 2, n_4\rangle\\ &+\delta_{i,j}\langle m_1m_2m_3 - 2, m_4|n_1n_2n_3 - 2, n_4\rangle\\ &-2\delta_{i,j}\langle m_1m_2m_3 - 2, m_4|N_{i,-1}|n_1n_2n_3 - 2, n_4\rangle.\end{aligned}$$

In a similar way one can treat progressively all the matrix elements of the two-body operators untill the recurrence relations are obtained.

The norm of the condensate state (3.5) is calculated in a similar way as has been explained for the systems with N=Z. The only difference is that now one needs to consider the matrix elements which involve the extra neutron pairs. They have, however, the same structure, as seen in the following example:

$$\begin{aligned}\langle m_1 m_2 m_3 m_4 | n_1 n_2 n_3 n_4 \rangle &= \textstyle\sum_i y_i \langle m_1 m_2 m_3 m_4 | P^+_{i,1} | n_1 n_2 n_3 n_4 - 1 \rangle \\ &= \textstyle\sum_i y_i \langle n_1 n_2 n_3 n_4 - 1 | P_{i,1} | m_1 m_2 m_3 m_4 \rangle^*.\end{aligned}$$

The recurrence relations are iterated starting from the matrix elements of the system with one pair. These matrix elements should be derived until they become analytical expressions in the mixing amplitudes x_i and y_i. We give here a few examples of such matrix elements involving a neutron pair in excess:

$$\begin{gathered}\langle - | P_{i,1} | 0001 \rangle = y_i, \\ \langle 0001 | T_{i,1} | 0100 \rangle = -x_i y_i, \quad \langle 0010 | T_{i,-1} | 0001 \rangle = x_i y_i, \\ \langle 1000 | N_{i,0} | 0001 \rangle = \langle 0001 | N_{i,0} | 0001 \rangle = 2 y_i^2.\end{gathered}$$

To evaluate the overlap of auxiliary states we need, in addition to the initial values already given in the previous chapter, the following matrix elements:

$$\langle 0001 | 1000 \rangle = \sum_i x_i y_i, \quad \langle 0001 | 0001 \rangle = \sum_i y_i^2.$$

The initial values for the matrix elements of the two-body operators, involving the extra neutron pair, are:

$$\begin{gathered}\langle 0001 | P^+_{i,1} P_{j,1} | 0001 \rangle = y_i y_j, \quad \langle 1000 | P^+_{i,1} P_{j,1} | 0001 \rangle = x_i y_j, \\ \langle 0010 | P^+_{i,0} P_{j,1} | 0001 \rangle = x_i y_j, \quad \langle 0001 | P^+_{i,1} P_{j,-1} | 0100 \rangle = x_j y_i.\end{gathered}$$

From the recurrence relations, using the initial values of the matrix elements, are obtained the average of the pairing Hamiltonian and the norm of the condensate. The mixing parameters x_i and y_i are then derived by minimizing the average of the Hamiltonian and imposing the normalization condition for the condensate state. The minimization is performed numerically, as explained in Appendix.

3.3 Application: coexistence of quartets and pairs in nuclei with N>Z

The QCM calculations presented here have a two-fold aim: to check the accuracy of QCM against exact shell model calculations and to study the competition between the quartet and pair correlations in nuclei with N>Z.

The calculations are done for nuclei with valence nucleons above the cores ^{16}O, ^{40}Ca and ^{100}Sn. Thus, we start with the N=Z isotopes studied in the previous chapter and then we add as many neutrons as can be treated exactly by shell model diagonalization. As in the case of N=Z nuclei, for the QCM calculations we use two inputs, based on spherical and deformed single-particle states.

Table 3.1: Correlation energies for *sd*-shell nuclei calculated with axially deformed single-particle states. The results are shown for the exact Shell Model (SM) diagonalization, the quartet condensate model and the PBCS1 approximation (Eq. 3.8). In brackets are given the errors relative to the exact SM results.

	Exact	QCM	PBCS1
^{20}Ne	6.550	6.539 (0.17%)	5.752 (12.18%)
^{22}Ne	6.997	6.969 (0.40%)	6.600 (5.67%)
^{24}Ne	7.467	7.426 (0.55%)	7.226 (3.23%)
^{26}Ne	7.626	7.592 (0.45%)	7.486 (1.84%)
^{28}Ne	7.692	7.675 (0.22%)	7.622 (0.91%)
^{30}Ne	7.997	7.994 (0.04%)	7.973 (0.30%)
^{30}Si	9.310	9.296 (0.15%)	9.064 (2.64%)
^{24}Mg	8.423	8.388 (0.41%)	7.668 (8.96%)
^{26}Mg	8.680	8.654 (0.30%)	8.258 (4.86%)
^{28}Mg	8.772	8.746 (0.30%)	8.531 (2.75%)
^{30}Mg	8.672	8.656 (0.18%)	8.551 (1.39%)
^{32}Mg	8.614	8.609 (0.06%)	8.567 (0.55%)
^{28}Si	9.661	9.634 (0.28%)	9.051 (6.31%)
^{32}Si	9.292	9.283 (0.10%)	9.196 (1.03%)

We shall present first the results obtained considering deformed single-particle states. They are obtained from deformed Skyrme-HF calculations with the Skyrme force SLy4 [50]. For the QCM calculations we chose again the lowest 7, 9 and 10 states above the cores mentioned above. The single-particle energies for neutrons and protons are considered to be equal (the Coulomb interaction is neglected in the mean field calculations) for all the isotopes, including the ones with N>Z. As shown in Ref. [2], the isospin dependence of the single-particle states can be eventually simulated with a term dependent on T^2, where T is the total isospin of the nucleus in the ground state. For the isovector pairing interaction we have taken a constant

strength force with $g = 24/A$.

The results obtained with the input presented above are shown in Tables 3.1 and 3.2. In these tables are given the correlation energies obtained with QCM, SM and PBCS1. The results for the approximation PBCS0 are not displayed here because they have much larger errors than PBCS1. This show again that at PBCS level the pn correlations are not properly taken into account. As can be seen in Tables 3.1 and 3.2, QCM predicts very accurately the correlation energies for all calculated isotopes. Thus, the errors remain below 1% even when many neutrons are added to the N=Z isotopes. From the fact that PBCS1 gives larger errors than QCM one concludes that the quartet correlations are not destroyed by the extra neutrons.

Table 3.2: The same results as in the previous Table, but for isotopes having as core ^{40}Ca and ^{100}Sn.

	Exact	QCM	PBCS1
^{44}Ti	3.147	3.142 (0.16%)	2.750 (12.61%)
^{46}Ti	3.526	3.509 (0.48%)	3.308 (6.18%)
^{48}Ti	3.882	3.853 (0.75%)	3.735 (3.79%)
^{50}Ti	3.973	3.956 (0.43%)	3.889 (2.11%)
^{104}Te	1.084	1.082 (0.18%)	0.964 (11.07%)
^{106}Te	1.324	1.321 (0.23%)	1.250 (5.59%)
^{108}Te	1.713	1.698 (0.88%)	1.642 (4.14%)
^{110}Te	1.892	1.880 (0.63%)	1.843 (2.59%)
^{48}Cr	4.248	4.227 (0.49%)	3.854 (9.27%)
^{50}Cr	4.461	4.444 (0.38%)	4.230 (5.18%)
^{52}Cr	4.743	4.721 (0.46%)	4.582 (3.39%)
^{54}Cr	4.869	4.855 (0.29%)	4.772 (1.99%)
^{108}Xe	1.870	1.863 (0.37%)	1.697 (9.25%)
^{110}Xe	2.191	2.185 (0.27%)	2.058 (6.07%)
^{112}Xe	2.449	2.437 (0.49%)	2.348 (4.12%)
^{114}Xe	2.964	2.954 (0.34%)	2.887 (2.60%)

To analyse how the accuracy of QCM depends on the input used for the isovector pairing Hamiltonian, we have also done calculations with spherical single-particle states and a pairing interaction extracted from the standard shell model calculations. This input was already presented in detail in the previous chapter. As an example of calculations done with this input, in Table 3.3 are given the results for the isotopes having as core ^{100}Sn. One can

notice that the accuracy of the QCM is similar to the one observed in the calculations based on a deformed mean field.

Table 3.3: Correlation energies for isotopes having as core ^{100}Sn calculated with spherical single-particle states.

	Exact	QCM	PBCS1
^{104}Te	3.831	3.829 (0.05%)	3.607 (5.85%)
^{106}Te	5.156	5.130 (0.50%)	4.937 (4.25%)
^{108}Te	5.970	5.930 (0.67%)	5.768 (3.38%)
^{110}Te	6.664	6.616 (0.72%)	6.485 (2.69%)
^{112}Te	6.815	6.764 (0.75%)	6.665 (2.20%)
^{108}Xe	6.752	6.696 (0.83%)	6.311 (6.53%)
^{110}Xe	7.578	7.509 (0.91%)	7.184 (5.20%)
^{112}Xe	8.285	8.208 (0.93%)	7.944 (4.12%)
^{114}Xe	8.446	8.368 (0.92%)	8.167 (3.30%)
^{116}Xe	8.031	7.947 (1.05%)	7.810 (2.75%)

An interesting issue is how fast the proton-neutron correlations are suppressed by adding extra neutron pairs. This information can be extracted from the proton-neutron pairing energy defined as $E^P_{np} = \langle g \sum_{i,j} P^+_{i,0} P_{j,0} \rangle$. How E^P_{np} evolves when one goes far from N=Z line by adding more neutrons is illustrated in Figs. 3.1 and 3.2 for the isotopes of Ne and Ti. The results correspond to the calculations presented in Tables 3.1 and 3.2. In the figures are plotted also the pairing energies for the protons and neutrons given by $E^P_{nn} = \langle g \sum_{i,j} P^+_{i,1} P_{j,1} \rangle$ and $E^P_{pp} = \langle g \sum_{i,j} P^+_{i,-1} P_{j,-1} \rangle$. It can be seen that, as expected, all the pairing energies are equal when N=Z. Then, by adding more neutrons the pn pairing energy is decreasing while the nn pairing energy is increasing. However, contrary to what it is generally believed, the pn correlations remain significantly large even for large number of extra neutron pairs.

To check further the accuracy of the QCM ansatz we have calculated also the occupation probabilities of the single-particle states for neutrons and protons. As an example, in Table 3.4 we show the occupation probabilities for the deformed single-particle states of ^{30}Mg. It can be noticed that the predictions of QCM for the occupation probabilities are very close to the exact results.

Finally, in order to understand better the correlations described by QCM, we have studied the entanglement properties of the collective pairs. The

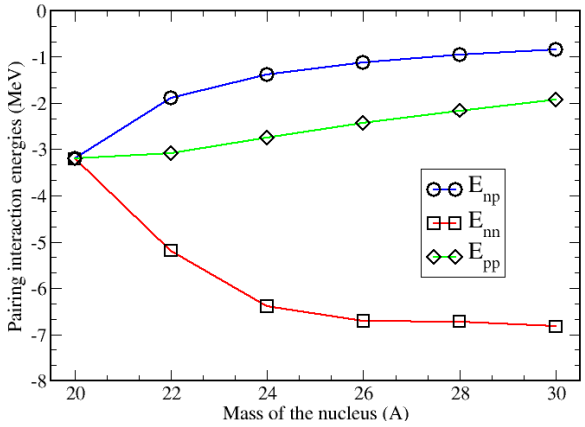

Figure 3.1: Proton-neutron, neutron-neutron and proton-proton pairing energies as a function of mass number for Ne isotopes. The results correspond to the calculations shown in Table 3.1.

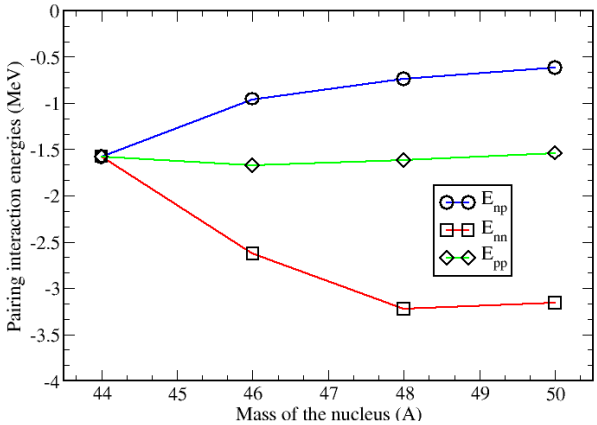

Figure 3.2: The same as in Fig. 3.1, but for Ti isotopes.

entanglement is measured with the so-called Schmidt number [51] defined by

$$K = (\sum_i w_i^2)^2 / \sum_i w_i^4, \tag{3.10}$$

where w_i are the amplitudes which define the two-body entanglement. In the case of pairing the mixing amplitudes are x_i and y_i. As an example we take the isotope ^{30}Mg, where the valence particles are distributed in two quartets and three neutron-neutron pairs. The Schmidt number for the protons inside the quartets, calculated with QCM, is $K = 1.88$. On the other hand, the Schmidt number for protons in the PBCS1 condensate is $K = 1.79$, showing that QCM is more effective in building correlations. For the neutrons in

Table 3.4: Occupation probabilities for neutrons (n) and proton (p) single-particle states in ^{30}Mg obtained by QCM and SM calculations.

ϵ_i	Exact(n)	QCM(n)	Exact (p)	QCM(p)
-16.45	0.995	0.995	0.983	0.983
-13.94	0.993	0.993	0.961	0.963
-10.39	0.987	0.987	0.028	0.026
-8.08	0.971	0.972	0.012	0.017
-6.09	0.921	0.923	0.007	0.007
-3.89	0.087	0.085	0.005	0.005
-2.61	0.045	0.045	0.004	0.004

excess the entanglement is stronger compared to the neutron pairs included in the quartets.

In conclusion, the results presented here and in the previous chapter show that QCM is able to describe with very high accuracy the pairing correlations induced by the isovector pairing in the ground state of $N \geq Z$ nuclei. This fact suggests that QCM can be used to describe accurately the isovector pairing in self-consistent mean-field calculations. In fact, combining Skyrme-HF and QCM we have proposed recently a calculation scheme for analyzing the role of isovector pairing on symmetry and Wigner energy [52].

Chapter 4

Quartet condensation for isovector and isoscalar pairing

4.1 Extension of QCM for treating isoscalar pairing

In open shell nuclei with N=Z are usually considered, in addition to isovector proton-neutron pairs, proton-neutron pairs with J=1. Since the proton-neutron pairs with J=1 should have T=0, they are commonly called isoscalar pairs. In principle one can form also isoscalar pairs with $J > 1$, but these pairs are expected to be less collective, except the particular case when neutrons and protons are sitted together in a partially filled high-degenerate state.

In many studies are discussed the isoscalar pairs with the total spin S=1 instead of J=1. The spin-triplet pairing S=1 is usually contrasted with the isovector spin-singlet S=0 pairing. This is a picture which is common for infinite systems. In nuclei one needs to take into account also the role played by the orbital angular momentum, L, of the pair. However, many calculations indicate that the pairing correlations are mainly generated by the L=0 part of the two-body interaction.

The question addressed in many studies is whether or not the isoscalar J=1 (or S=1) pairing does really exist in N=Z nuclei and, if so, how it does compete with the isovector pairing. These issues are commonly studied in the framework of generalized BCS or HFB theories, summarized in Chapter I. As pointed out in some studies [14], the competition between the isovector and isoscalar pairing described by BCS/HFB models appears to be affected significantly by the non-conservation of particle number.

In this chapter we shall treat the isovector and the isoscalar pairing in a

quartet model similar to the one we have used for the treatment of isovector pairing. The model will be formulated for the description of the ground state of the isovector-isoscalar pairing Hamiltonian

$$\hat{H} = \sum_i \epsilon_i (N_i^\nu + N_i^\pi) + \sum_{i,j} V_{ij}^{(T=1)} \sum_\tau P_{i,\tau}^+ P_{j,\tau} + \sum_{i,j} V_{ij}^{(T=0)} \sum_\sigma D_{i,\sigma}^+ D_{j,\sigma}. \quad (4.1)$$

In the first term ϵ_i are the single-particle energies for protons and neutrons, supposed to be equal in N=Z systems (as usual, the Coulomb interaction is neglected) while N_i^ν and N_i^π are, respectively, the operators for the neutron and proton numbers. The second term is the isovector interaction, discussed in the previous chapters, and the last term is the isoscalar pairing interaction (T=0). As we have mentioned above, the isoscalar pairing can be considered for S=1 or J=1 pairs. For the case of S=1 pairs the operators D appearing in the last term of the Hamiltonian are given by

$$D_{i,\sigma}^+ = [a_i^+ a_{\bar{i}}^+]_{l=0,\ \sigma,\ \tau=0}^{L=0,\ S=1,\ T=0}. \quad (4.2)$$

When the isoscalar pairs have J=1, the pairing operator is

$$D_{i,M}^+ = [a_i^+ a_{\bar{i}}^+]_{M,\ \tau=0}^{J=1,T=0}. \quad (4.3)$$

This operator is the analogous of the isovector pair operator

$$P_{i,\tau}^+ = [a_i^+ a_{\bar{i}}^+]_{M=0,\ \tau}^{J=0,\ T=1}. \quad (4.4)$$

As can be seen, the isovector and the isoscalar pair operators have formally the same structure and can be interchanged by replacing the isospin with the spin. This symmetry is used below for extending the quartet model to the isoscalar pairing.

The formal analogy between the isovector and isoscalar pairing can be seen better for double-degenerate levels, e.g., spherical single-particle levels with j=1/2 or axially deformed single-particle levels. In such a case the isovector and the isoscalar operators are given by:

$$P_{i,+1}^+ = \nu_i^+ \nu_{\bar{i}}^+, \quad P_{i,-1}^+ = \pi_i^+ \pi_{\bar{i}}^+, \quad (4.5)$$

$$P_{i,0}^+ = \frac{1}{\sqrt{2}} (\nu_i^+ \pi_{\bar{i}}^+ + \pi_i^+ \nu_{\bar{i}}^+), \quad (4.6)$$

$$D_{i,+1}^+ = \nu_i^+ \pi_i^+, \quad D_{i,-1}^+ = \nu_{\bar{i}}^+ \pi_{\bar{i}}^+, \quad (4.7)$$

$$D_{i,0}^+ = \frac{1}{\sqrt{2}} (\nu_i^+ \pi_{\bar{i}}^+ - \pi_i^+ \nu_{\bar{i}}^+). \quad (4.8)$$

From the equations above one can grasp immediately the formal analogy between the isovector and the isoscalar pairs.

In the case of isovector pairing the quartets have been introduced as a simple manner to construct wave functions with the total isospin T=0 from isovector pairs of T=1. For isoscalar pairing we employ a similar procedure to construct a wave function of total J=0 from isoscalar pairs of J=1. Thus, using this analogy we define the non-collective isoscalar quartet operators

$$B^+_{ij} = [D^+_i D^+_j]^{J=0}. \tag{4.9}$$

With this operators we construct a collective isoscalar quartet:

$$B^+ = \sum_{i,j} x_{ij} B^+_{ij}. \tag{4.10}$$

As in the isovector case, we make the assumption that the mixing amplitudes are separable in the indices i and j. It can be easily seen that in this case the collective isoscalar quartet can be written as

$$B^+ = 2\Delta^+_1\Delta^+_{-1} - (\Delta^+_0)^2, \tag{4.11}$$

where Δ are the collective isoscalar pair operators

$$\Delta^+_M = \sum_i x_i D^+_{i,M}. \tag{4.12}$$

We can thus see that the collective isoscalar quartets have formally the same structure as the isovector quartets.

Finally, we suppose that the isovector and the isoscalar pairing correlations can be described by the quartet condensate:

$$|\Psi\rangle = (\alpha A^+ - \beta B^+)^{n_q}|0\rangle. \tag{4.13}$$

It can be observed that now the quartet which is used to construct the condensate is taken as a linear superposition between the isovector and the isoscalar quartets. As a consequence, the wave function becomes a nontrivial superposition of isovector and isoscalar condensates. This can be seen by writing explicitely the binomial expansion in Eq. (4.13):

$$|\Psi\rangle = (\alpha A^+ - \beta B^+)^{n_q}|0\rangle = \textstyle\sum_{k=0}^{n_q}\sum_{k'=0}^{n_q-k}\sum_{k''=0}^{k}(-)^{(k+k'+k'')}2^{(n_q-k'-k'')}$$

$$\cdot C^k_n C^{k'}_{n-k} C^{k''}_k \cdot \alpha^{(n-k)}\beta^k \cdot (\Gamma^+_1\Gamma^+_{-1})^{(n-k-k')}(\Gamma^+_0)^{2k'}(\Delta^+_1\Delta^+_{-1})^{(k-k'')}(\Delta^+_0)^{2k''}|0\rangle. \tag{4.14}$$

The condensate (4.13) depends on the mixing amplitudes x_i which measure the collectivity of the pair operators. It should be noticed that, due to the symmetry between the isospin and spin degrees of freedom and because we treat here N=Z systems, the isovector and isoscalar pairs are described by the same mixing amplitudes. In addition, the condensate depends on the parameters α and β, which take into account the mixing between the isoscalar and isovector correlations. Using the normalization of the wave function, one can take $\alpha = \sqrt{1-\beta^2}$. The amplitudes x_i and the parameter β are determined variationally from the minimization of the average of the Hamiltonian (4.1). The average is calculated with the method of recurrence relations which is described in the next section.

4.2 Solution of QCM equations for isovector and isoscalar pairing

To calculate the average of the isovector-isoscalar pairing Hamiltonian and the norm of the quartet condensate we use the auxiliary states:

$$|n_1 n_2 n_3,\ m_1 m_2 m_3\rangle = \Gamma_1^{+n_1}\Gamma_{-1}^{+n_2}\Gamma_0^{+n_3}\Delta_1^{+m_1}\Delta_{-1}^{+m_2}\Delta_0^{+m_3}|0\rangle. \tag{4.15}$$

The states above depend on 6 parameters which count all types of isovector and isoscalar pairs. For the calculations we consider all the possible combinations of the 6 parameters compatible with the total number of pairs.

The calculation scheme is similar to the one used for the isovector pairing. Thus, we calculate first all the relevant commutation relations between the basic operators which define the Hamiltonian. In fact, in order to close the commutation relations between the pair operators one needs all the operators of SO(8) algebra associated with the isovector-isoscalar Hamiltonian. Thus, one needs to consider, in addition to the operators we have used in the case of isovector pairing, the operators

$$S_{i,M} = [a_i^+ a_i]^{J=1,\,T=0}_{M,\tau=0}, \tag{4.16}$$

$$W_{M,\tau} = [a_i^+ a_i]^{J=1,T=1}_{M,\ \tau}. \tag{4.17}$$

The necessity of introducing the operators W can be seen from the commutation relations between the isovector and isoscalar pair operators:

$$[D_{i,M}, P^+_{j,\tau}] = (-)\delta_{ij}(-)^M W_{-M,\tau}. \tag{4.18}$$

In order to calculate the action of the pair operators on the auxiliary states one needs also to consider the commutators:

$$[W_{i,M,\tau}, P^+_{j,\tau'}] = \delta_{ij}\delta_{\tau,-\tau'}(-)^\tau D^+_{i,M}, \tag{4.19}$$

and

$$[W_{i,M,\tau}, D^+_{j,M'}] = \delta_{ij}\delta_{M,-M'}(-)^M P^+_{i,\tau}. \tag{4.20}$$

The commutation relations involving the spin operator S are similar to the ones for the isospin operator T, which are given in Chapter II.

Using the commutation relations for the SO(8) algebra one calculates the action of the basic operators on the auxiliary states. How the calculations can be done is illustrated below. Thus, the action of the pair operator $P_{i,1}$ on the auxiliary states can be written as:

$$P_{i,1}|n,m\rangle = P^{(n)}_{i,1}|n,m\rangle + P^{(m)}_{i,1}|n,m\rangle - \frac{1}{2}n_1 x_i N^{(m)}_{i,0}|n_1 - 1 n_2 n_3, m\rangle. \tag{4.21}$$

The index (n) or (m) on the operators denotes the fact that they act only on the isovector states $|n\rangle \equiv |n_1 n_2 n_3\rangle$ or only on the isoscalar states $|m\rangle \equiv |m_1 m_2 m_3\rangle$. The action of $P_{i,1}$ on the $|n\rangle$ states is already known and it was given in Chapter II. The action of $P_{i,1}$ on the isoscalar states $|m\rangle$ is given by:

$$P_{i,1}|m\rangle = -m_1 m_2 x_i^2 P^+_{i,-1}|m_1 - 1 m_2 - 1 m_3\rangle + \frac{m_3(m_3-1)}{2}x_i^2 P^+_{i,0}|m_1 m_2 m_3 - 2\rangle. \tag{4.22}$$

It remains to write down the action of $N_{i,0}$ on the isoscalar states, which is given by:

$$N_{i,0}|m\rangle = 2m_3 x_i D^+_{i,0}|m_1 m_2 m_3 - 1\rangle + 2m_1 x_i D^+_{i,1}|m_1 - 1 m_2 m_3\rangle$$
$$+2m_2 x_i D^+_{i,-1}|m_1 m_2 - 1 m_3\rangle. \tag{4.23}$$

We consider now the action of $D_{i,1}$ on the auxiliary states:

$$D_{i,1}|n,m\rangle = D^{(n)}_{i,1}|n,m\rangle + D^{(m)}_{i,1}|n,m\rangle - \frac{1}{2}m_1 x_i N^{(n)}_{i,0}|n, m_1 - 1 m_2 m_3\rangle. \tag{4.24}$$

The action of $D_{i,1}$ on the isovector states is similar to the action of $P_{i,1}$ on the isoscalar states and can be written as:

$$D_{i,1}|n\rangle = -n_1 n_2 x_i^2 D^+_{i,-1}|n_1 - 1 n_2 - 1 n_3\rangle + \frac{n_3(n_3-1)}{2}x_i^2 D^+_{i,-1}|n_1 n_2 n_3 - 2\rangle. \tag{4.25}$$

The action of $D_{i,1}$ on the isoscalar states is again similar with the action of $P_{i,1}$ on the isovector states, and has the expression:

$$D_{i,1}|m\rangle = -\tfrac{m_3(m_3-1)}{2}x_i^2 D^+_{i,-1}|m_1 m_2 m_3 - 2\rangle + m_1 x_i|m_1 - 1 m_2 m_3\rangle$$
$$-m_1 m_3 x_i^2 D^+_{i,0}|m_1 - 1 m_2 m_3 - 1\rangle - m_1(m_1-1)x_i^2 D^+_{i,1}|m_1 - 2 m_2 m_3\rangle.$$

The action of $N_{i,0}$ on the isovector states $|n\rangle$ is already known from Chapter II.

In a similar way we calculate the action of the operators S and W. Some of these expressions are given below.

$$S_{i,1}|m\rangle = -m_2 x_i D^+_{i,0}|m_1 m_2 - 1 m_3\rangle - m_3 x_i D^+_{i,1}|m_1 m_2 m_3 - 1\rangle, \quad (4.26)$$

$$W_{0,0}|n,m\rangle = m_3 x_i P^+_{i,0}|n, m_1 m_2 m_3 - 1\rangle + n_3 x_i D^+_{i,0}|n_1 n_2 n_3 - 1, m\rangle, \quad (4.27)$$

$$W_{1,1}|n,m\rangle = -n_2 x_i D^+_{i,1}|n_1 n_2 - 1 n_3, m\rangle - m_2 x_i P^+_{i,1}|n, m_1 m_2 - 1 m_3\rangle, \quad (4.28)$$

$$W_{-1,-1}|n,m\rangle = -n_1 x_i D^+_{i,-1}|n_1 - 1 n_2 n_3, m\rangle - m_1 x_i P^+_{i,-1}|n, m_1 - 1 m_2 m_3\rangle. \quad (4.29)$$

Having all the expressions for the action of the basic operators on the auxiliary states we calculate the matrix elements of the pairing interaction. Below we illustrate this calculation for the matrix element $\langle n', m'|D^+_{i,1}D_{j,1}|n,m\rangle$. Thus, first we act with $D_{j,1}$ on the right hand side, we write all the terms which come out of it, then we continue by acting with the operator $D^+_{i,1}$ on the left hand side. In this way one generates many terms which are calculated by applying the same procedure. How this can be done we illustrate for the following term:

$$\begin{gathered}
\langle n', m'|D^{+(m')}_{i,1}D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle = \\
-\tfrac{m'_3(m'_3-1)}{2} x_i^2 \langle n', m'_1 m'_2 m'_3 - 2|D_{i,-1}D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle \\
+m'_1 x_i \langle n', m'_1 - 1 m'_2 m'_3|D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle \\
-m'_1 m'_3 x_i^2 \langle n', m'_1 - 1 m'_2 m'_3 - 1|D_{i,0}D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle \\
-m'_1(m'_1 - 1) x_i^2 \langle n', m'_1 - 2 m'_2 m'_3|D_{i,1}D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle.
\end{gathered}$$

The first, the third and the fourth terms in the righ hand side should be further changed in order to get matrix elements for two-body operators D^+D. Thus, the third term becomes:

$$\begin{gathered}
\langle n', m'_1 - 1 m'_2 m'_3 - 1|D_{i,0}D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle = \\
\langle n_1 - 1 n_2 - 1 n_3, m|D^+_{i,0}D_{j,-1}|n', m'_1 - 1 m'_2 m'_3 - 1\rangle \\
-\delta_{ij}\langle n', m'_1 - 1 m'_2 m'_3 - 1|S_{i,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle.
\end{gathered}$$

The recurrence relations involve also the matrix elements for the products of isovector and isoscalar pair operators. They are essentially generated by the matrix elements of the products between the particle number and pair operators. An example is given below:

$$\langle n', m'_1 - 1 m'_2 m'_3|N^{(n')}_{i,0}D^+_{j,-1}|n_1 - 1 n_2 - 1 n_3, m\rangle =$$

$$2n'_3x_i\langle n'_1n'_2n'_3-1,m'_1-1m'_2m'_3|P_{i,0}D^+_{j,-1}|n_1-1n_2-1n_3,m\rangle$$
$$2n'_1x_i\langle n'_1-1n'_2n'_3,m'_1-1m'_2m'_3|P_{i,1}D^+_{j,-1}|n_1-1n_2-1n_3,m\rangle$$
$$2n'_2x_i\langle n'_1n'_2-1n'_3,m'_1-1m'_2m'_3|P_{i,-1}D^+_{j,-1}|n_1-1n_2-1n_3,m\rangle.$$

To obtain in the terms above the matrix elements of the operators D^+P, one needs to interchange the order of the pair operators, which can be done using the commutation relations between them. Thus, for the first term one gets:

$$\langle n'_1n'_2n'_3-1,m'_1-1m'_2m'_3|P_{i,0}D^+_{j,-1}|n_1-1n_2-1n_3,m\rangle =$$
$$\langle n'_1n'_2n'_3-1,m'_1-1m'_2m'_3|D^+_{j,-1}P_{i,0}|n_1-1n_2-1n_3,m\rangle$$
$$-\delta_{ij}\langle n'_1n'_2n'_3-1,m'_1-1m'_2m'_3|W_{i,-1,0}|n_1-1n_2-1n_3,m\rangle.$$

We stop here the illustration of the recurrence relations for isovector-isoscalar pairing calculations. As can be observed from the examples presented above, they are much more complicated than the recurrence relations for isovector pairing.

We end this section by providing some of the initial values of the matrix elements which are needed to iterate the recurrence relations for isovector-isoscalar pairing. For the auxiliary states with zero pairs we use the notation $|-\rangle = |n_1=0,n_2=0,n_3=0;m_1=0,m_2=0,m_3=0\rangle$. The notation "-" is used also to indicate zero isovector or isoscalar pairs.

First, we show explicitely how to get the initial matrix elements for the operator D_0. Thus, for a state with an isoscalar pair $m_3=1$ one gets:

$$\langle -,-|D_{i,0}|-,001\rangle = \langle -,-|[D_{i,0},\Delta^+_0]|-,-\rangle = \textstyle\sum_j x_j\langle -,-|[D_{i,0},D^+_{j,0}]|-,-\rangle$$
$$= \textstyle\sum_j x_j\langle -,-|\delta_{ij}(1-\frac{1}{2}N_{i,0})|-,-\rangle$$
$$= \textstyle\sum_j x_j\delta_{ij}\langle -,-|-,-\rangle - \sum_j x_j\frac{1}{2}\langle -,-|N_{i,0}|-,-\rangle = x_i.$$

In the same way we have calculated the initial values for the matrix elements of other basic operators. The results are:

$$\langle -,-|D_{i,1}|-,100\rangle = \langle -,-|D_{i,-1}|-,010\rangle = x_i,$$

$$\langle -,001|S_{i,1}|-,010\rangle = \langle -,100|S_{i,1}|-,001\rangle = -x_i^2,$$

$$\langle -,001|N_{i,0}|-,001\rangle = \langle -,010|N_{i,0}|-,010\rangle = \langle -,100|N_{i,0}|-,100\rangle = 2x_i^2,$$

$$\langle -,100|W_{i,1,1}|010,-\rangle = \langle -,010|W_{i,-1,-1}|100,-\rangle = -x_i^2,$$

$$\langle 001,-|W_{i,0,0}|100,-\rangle = x_i^2.$$

Finally, we give the initial values for some two-body operators which enter in the definition of the pairing interaction:

$$\langle -,001|D^+_{i,0}D_{j,0}|-,001\rangle = \langle 001,-|P^+_{i,0}P_{j,0}|001,-\rangle = x_i x_j.$$

Providing all the initial values of the matrix elements one can get, recursively, the average of the Hamiltonian. The mixing amplitudes x_i and the parameter β, which express the contribution of the isoscalar quartets, are calculated variationally from the minimization of the Hamiltonian average and from the norm of the quartet condensate.

4.3 Application: competition between isovector and isoscalar pairing in N=Z nuclei

With the QCM formalism presented above we have studied the competition between the isovector and the isoscalar pairing in N=Z nuclei. As an example, we present the calculations done for ^{44}Ti and ^{48}Cr. In these calculations are taken into account the valence nucleons moving in the pf-shell, above the closed core ^{40}Ca. The isovector and the isoscalar pairing interactions have been extracted from the (J=0,T=1) and (J=1,T=0) part of the monopole-modified Kuo-Brown interaction (KB3G).

Table 4.1: Correlation energies for ^{44}Ti and ^{48}Cr calculated with the isovector-isoscalar pairing Hamiltonian. In the brackets are given the errors of the QCM results in comparison with the exact SM calculations. The last column shows the values of the parameter β, which indicates the contribution of the isoscalar correlations.

Nuclei	Shell Model	Quartets (errors)	β^2
^{44}Ti	4.261	4.221 (0.38 %)	0.0094
^{48}Cr	6.303	6.271 (0.50 %)	0.075

The results for the pairing correlation energies and for the amplitude β are given in Table 4.1. First, one can see that the condensate model gives very accurate results compared to the exact shell model calculations. Second, it can be noticed that for both isotopes the parameter β is very small, indicating a very small contribution of the isoscalar pairing correlations to

the wave function. As shown in some studies (e.g., see [53, 54]) the isoscalar pairing force gives small pairing correlations because it is suppressed by the spin-orbit interaction.

Table 4.2: Correlation energies for pf-shell nuclei calculated with the isovector-isoscalar pairing Hamiltonian and using in QCM only the isovector quartet.

Nuclei	Shell Model	Quartets (errors)
^{44}Ti	4.261	4.169 (2.2 %)
^{48}Cr	6.303	6.119 (2.9 %)
^{52}Fe	5.978	5.737 (4.0 %)

To see how important is the contribution of the isoscalar pairing correlations in these nuclei, we have also performed QCM calculations neglecting the contribution of the isoscalar quartet in the quartet condensate state, i.e., taking $\beta = 0$. The results are presented in Table 4.2. It can be seen that the errors compared to SM remain resonably small. This fact demonstrates that, in the first approximation, the isoscalar pairing correlations can be neglected in pf-shell nuclei with N=Z.

Finally, we would like to stress the fact that the calculations presented in this chapter are done with the isoscalar pairs built by time-reversed state. However, isoscalar J=1 pairs can be also constructed with neutrons and protons belonging to single-particle states which are not time-reversed. How much these pairs are contributing in the ground state of N=Z nuclei is an interesting subject we are presently investigating [55].

Summary and conclusions

In this thesis we have discussed the theoretical treatment of proton-neutron pairing in atomic nuclei. We have started by a short review of the BCS-like models which are commonly used to describe proton-neutron correlations in nuclei. Taking as an example the treatment of isovector pairing by BCS and PBCS models, we have emphasized that these models are not able to describe properly the proton-neutron correlations, mainly due to the fact that they break the isospin invariance. Then, in the next chapters we have presented the main results of our PhD studies. Thus, in Chapter II we have introduced our approach for the treatment of the isovector pairing correlations, which, in contrast to the BCS-type models, conserves exactly the particle number and the isospin. In this approach, called quartet condensation model (QCM), the isovector pairing correlations in N=Z nuclei are described in terms of alpha-like quartets formed by two isovector pairs coupled to the total isospin T=0. The ground state is built as a condensate of the collective alpha-like quartet, i.e., by applying the same quartet operator many times, according to the number of quartets which can be formed with the valence neutrons and neutrons. The quartet condensate model is applied for N=Z nuclei with valence nucleons outside the cores ^{16}O, ^{40}Ca and ^{100}Sn. The QCM calculations are done first with single-particle energies and isovector pairing interactions extracted from commonly used shell model (SM) forces. The comparison with exact SM calculations shows that QCM gives a very accurate description of the isovector pairing correlations in N=Z nuclei. Thus, for all calculated isotopes, the errors for the pairing correlation energies are less than 1%. The same high accuracy we have obtained for the QCM calculations done with an input corresponding to an axially deformed mean field, which takes into account, in an effective way, the quadrupole degree of freedom, important in N=Z nuclei.

Next, in Chapter III we have extended the QCM approach in order to treat N>Z nuclei. For these nuclei we considered a ground state formed by a product of two condensates, one of quartets and the other of neutron pairs in excess relative to the proton pairs. It is shown that this ansatz gives a

very accurate description of the isovector pairing correlations in N>Z nuclei, better than the PBCS models based on a product of neutron and proton pairs. This indicates that the quartets do coexist with the neutron pairs in N>Z nuclei. In particular, the QCM calculations show that the proton-neutron pairing correlations remain important when one goes away from N=Z line, which is contrary to what BCS calculations usually predict.

In the last chapter we have presented how the QCM approach is extended to take into account both the isovector and the isoscalar pairing correlations. Using the analogy suggested by the spin-isospin symmetry, the isoscalar pairing is described by a quartet formed by coupling two isoscalar pairs with J=1 to a total J=0. Then, we have introduced a generalized quartet formed by a linear combination of isoscalar and isovector quartets. With the generalized quartet we constructed a quartet condensate which we have further used to describe the competition between the isoscalar and the isovector pairing in N=Z nuclei. As an illustration we have considered the isotopes ^{44}Ti and ^{48}Cr. The comparison with exact SM calculations shows that the extended QCM describes with a very high accuracy the isovector-isoscalar pairing correlations. For these isotopes the QCM calculations show also that in these nuclei the isoscalar pairing correlations play a minor role in comparison with the isovector pairing correlations. This conclusion should be further checked by including in the calculations the isoscalar proton-neutron pairs built on states which are not time-reversed. However, these additional pairs are not expected to change much the present results: since, as shown in some recent studies [53, 54], the isoscalar pairing is strongly suppressed by the spin-orbit interaction.

Finally we would like to make a few clarifying comments relative to the quartet condensation model which we have used in our thesis. Here the name " quartet condensate" is used in the same sense as it is used "pair condensate" in BCS theory, namely as a state formed by applying many times the same quartet operator. Since the quartet operator is not a boson, the quartet condensate is not a bosonic condensate. In addition, should be kept in mind that the alpha-like quartet is not describing an alpha particle (^{4}He) localized in the space. Alpha-like quartet means here a four-body structure of two neutrons and two protons correlated in spin and isospin and not necessarily in coordinate space.

It is also worth mentioning that in all the calculations presented in this thesis we focused only on the pairing part of the two-body interaction. Thus, when we compare QCM with the SM calculations, the latter refer in fact to the exact diagonalization of the pairing interactions and not to the calculations done with the full shell model interaction. Therefore the QCM has to be used as are commonly used the BCS-type models, i.e., for treating only

the effects induced by the pairing interaction. The other very important degrees of freedom, such as quadrupole, can be eventually taken into account through the mean field approximation, e.g., as usually done in HF+BCS calculations. In fact, using the analogy with the HF+BCS calculations, we have designed recently a HF+QCM calculation scheme for taking into account the influence of proton-neutron pairing correlations on ground state properties of nuclei with protons and neutrons moving in the same valence shell [52].

Appendix: Numerical solution of QCM equations

The QCM calculations require the determination of the parameters which define the quartet condensate function. These parameters are the mixing amplitudes of the collective pairs and they are determined variationally. Thus, denoting by $|\Psi(x)\rangle$ the QCM state and by x the variational parameters, one needs to perform the minimization of the functional

$$E(x) = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{4.30}$$

where $\hat{H}$ is the pairing Hamiltonian. The minimization should be done by imposing the normalization condition, i.e., $N(x) = \langle\Psi|\Psi\rangle = 1$.

The main difficulty of QCM calculations is to obtain analytically the average of the Hamiltonian as a functional of the parameters x. As explaind in Chapters II-IV, this task is performed by using the method of recurrence relations. The derivation of the recurrence relations is long and not trivial, especially for the case of isovector-isoscalar pairing. Once derived analytically, the recurrence relations are included in the numerical code together with the initial matrix elements necessary to start the iteration procedure.

To do the minimization we have employed the subroutine E04UCF extracted from NAG library [56]. This subroutine is called in the following form:

$$call\ e04ucf(nx, nclin, ncnln, lda, ldcj, ldr, a, bl, bu, confun, objfun, iter,$$
$$istate, c, cjac, clambda, objf, objgrd, r, x, iwork, liwork, work, lwork,$$
$$iuser, user, ifail).$$

where $x(n_x)$ is a vector of dimension n_x which stores the variational parameters. $objfun$ is a function which returns, for a given x, the average of the Hamiltonian, $E(x)$, while $confun$ is the function which returns the value of the norm $N(x)$. The subroutine provides the variational parameters determined with the required precision.

The arhitecture of the code is quite complex because one needs to store in an efficient way the matrix elements of all basic operators which define the SO(5) or SO(8) algebras, associated to the isovector and isovector-isoscalar pairing Hamilonians, together with the matrix elements of the pairing interactions. As explained in Chapters II-IV, the calculations are done in the basis of auxiliary vectors defined for an arbitrary number of collective pairs. Thus, for the isovector-isoscalar pairing the auxiliary vectors depend on 6 variables, i.e., $|n_1n_2n_3, m_1m_2m_3\rangle$. In order to keep track of the matrix elements of the operators in this basis, we need to calculate all the possible configurations compatible with a given number of total pairs, i.e., $n = n_1 + n_2 + n_3 + m_1 + m_2 + m_3$. This job is done in the first subroutine of the code. In the next subroutine we calculate the recurrence relations for the basic operators, i.e., P, D, N, T, S and W (see the notations in Chapters II-IV) together with the recurrence relations for the norm. The third subroutine contains the recurrence relations for the two-body operators P^+P and D^+D, as well as the matrix elements for all the combinations between these operators. In the following subroutine are calculated, in terms of the matrix elements of the auxiliary states, the average of the Hamiltonian and the norm of the quartet condensate function. These results are then used to construct the function "objun" and "confun" called by the subroutine which does the minimization.

The code, which contains a few thousand lines in the case of isovector-isoscalar pairing, was tested using exactly solvable models for the pairing problem. More precisely, we verified the code in the case of degenerate levels, for which the pairing problem can be solved exactly.

Finally we would like to mention that, in spite of its complexity, the code is running quite fast. For example, to calculate the ground state energy of a nucleus with N=Z it takes a few minutes on an ordinary laptop.

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